OAK RIDGE
NATIONAL LABORATORY
MANAGED BY UT-BATTELLE
FOR THE DEPARTMENT OF ENERGY

ORNL/TM-9179/R5
ENDF-364

Updated Users' Guide for SAMMY Multilevel R-matrix Fits to Neutron Data Using Bayes' Equation

Nancy M. Larson

November 2000

UT-BATTELLE
ORNL-27 (4-00)

ORNL/TM-9179/R5
ENDF-364

Computational Physics and Engineering Division

UPDATED USERS' GUIDE FOR SAMMY: MULTILEVEL R-MATRIX FITS TO NEUTRON DATA USING BAYES' EQUATION

Nancy M. Larson

Date Published: August 1984
Date of Revision 1: April 1985
Date of Revision 2: June 1989
Date of Revision 3: September 1996
Date of Revision 4: December 1998
Date of Revision 5: October 2000

Prepared by the
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831
managed by
UT-Battelle, LLC
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-00R22725

CONTENTS

LIST OF TABLES

LIST OF FIGURES

ACKNOWLEDGMENTS FOR REVISION 5

The encouragement and support of SAMMY users is gratefully acknowledged. I am indebted first to ORNL researchers (Luiz Leal, Herve Derrien, Royce Sayer, Klaus Guber, Paul Koehler) and then to outside users (Frank Gunsing, Olivier Bouland, Soo Youl Oh, Kun Joong Yoo, Greg Leinweber, Yaron Danon) for their helpful suggestions and for their skill in uncovering my programming errors. Royce Sayer's work was invaluable in adding the Coulomb capability to the code. Special thanks must go to Ali Nouri of NEA, Paris, for organizing the SAMMY workshop held in September of 1999 and for maintaining the website at http://www.nea.fr/html/dbdata/sammy.htm. Finally, my apologies to the many SAMMY users whose names are not mentioned here, but whose contributions are important to the development and maintenance of this code.

ABSTRACT FOR REVISION 5

Modifications and new features of the resonance analysis code SAMMY, release M5, are documented in Revision 5 of the SAMMY Users' Guide. Among the new features added to the code are: (1) The capability to generate Coulomb penetrabilities and shift factors, so that charged particles can be used either in final states or as the incident particle. (2) Modernization of the code's structure, resulting in increased computation speed. (3) Improved treatment of the Unresolved-Resonance Region. (4) Bondarenko averaging. (5) Compliance with new ENDF formats for File 2 (Reich-Moore resonance parameters). (6) Generalization of the RPI resolution function. A more complete listing of the new and improved features available in M5 is given in the Introduction to Revision 5.

INTRODUCTION TO REVISION 5

Modifications and improvements to SAMMY subsequent to the publication of Revision 4 of this manual are summarized here.

(1) The ability to calculate Coulomb penetrabilities, shift factors, and phase shifts will extend the applicability of SAMMY to other types of data such as (n,α), (n,p), (p,n), (α,n). Section III.H provides details on the Coulomb implementation in SAMMY.

(2) One change which is essentially invisible to the SAMMY user is the combination of the various segments into one large program. In addition to easing portability problems, this change has resulted in increased computation speed; SAMMY runs with Version M5 will require less CPU time than the same runs with earlier versions. Details are found in Sect. XI.

(3) From the equations for Doppler broadening (Sect. IV.A.1 and IV.F), it is clear that the Doppler width is mass-dependent, and therefore changes from nuclide to nuclide. Unfortunately this detail was overlooked in prior versions of SAMMY (M2a and earlier). That oversight has been corrected for Version M5. For most experimental conditions, this will be a small effect. For cases in which two nuclides, both with large abundances, have vastly different masses, the effect will be more pronounced. SAMMY users will want to be aware of this error, and consider what impact it might have on their evaluations.

(4) It is now possible to calculate individual reaction types or individual fission channels. For example, one might wish to know the (n,α) cross section separately from (n,p) or (n,n'). [In prior versions of SAMMY, all "exit channels" were automatically included in the outgoing final state whenever the data was specified as inelastic, fission, or reaction.] Details on how this is accomplished are given in Sect. V.L, page 98w.

(5) A bug was discovered (and exterminated) in the derivatives with respect to resonance parameters. This bug was found while the author was playing with artificial data, and occurred only when the penetrability was very small, that is for low energies and non-zero angular momentum. Hence it is highly unlikely to have affected calculations relating to physical data.

(6) Errors in implementation of the RPI resolution function have been corrected, and the form of the function generalized. Preliminary values of resolution parameters suitable for use with Geel data are provided. See Sect. IV.G.

(7) Values of parameters for either the RPI resolution function or the ORR resolution function can now be given in either the INPut file or the PARameter file. If any parameter is to be varied, the PARameter file must be used.

(8) Improvements in the treatment of the Unresolved-Resonance Region include more exact calculation of partial derivatives, normalization options for the experimental data, and increased flexibility for input of experimental data. Details are given in Section V.J (page 98s).

(9) Derivatives with respect to the matching radius (channel radius) are now generated in a self-consistent and logical manner. When the matching radius is varied but the neutron width is held fixed, the width Γ_n and not the partial width amplitude γ_n remains unchanged. This is true also for other widths with non-unit penetrabilities (including Coulomb penetrabilities).

(10) It is now possible to utilize the MPW solution for Bayes' Equations in the resolved resonance region in a limited fashion. Individual SAMMY runs can generate W_i and Y_i for several data sets, and an additional SAMMY run will read those arrays, add them appropriately, and update the parameter values and covariance matrix (i.e., solve Bayes' equations via MPW method). See Sect. II.B.1.c (page 20c) for more details. This scheme was initially devised for retroactively generating an approximate covariance matrix for a pre-existing set of resonance parameters.

(11) Bondarenko averaging is now available for the generation of multigroup cross sections; see Sect. V.C.2 for details.

(12) Output covariance matrices for the resonance parameters can now be provided in an abbreviated "concise" ASCII file, which the author intends to propose for adoption as an ENDF format. Details are given in Section VII.E.

(13) SAMMY can utilize ENDF File 2 (LRU=1, LRF=3, i.e. the Reich-Moore format) for input of resonance parameters (see Sect. VI.G), and can also provide output in ENDF File 2 format (see Sect. VI.F). The format change approved at the November, 1999, CSEWG meeting is included; this format change permits specification of channel spin as well as resonance spin and orbital angular momentum for each resonance.

(14) Additional output files, in legible (ASCII) format, is now provided by the auxiliary programs SAMORT (Sect. VIII.C) and SAMRPT (Sect. VIII.M). These new files, with extensions PLT, are intended for use where the ORNL plotting package FORODF is replaced by another package.

(15) Auxiliary code SAMSMC can be used to generate Monte-Carlo simulations of the multiple-scattering corrections to capture and/or fission yields. See Sect. VIII.O page 150z.7.

II. BAYES' EQUATIONS

Starting from Bayes' theorem and three basic assumptions, one can derive formulae for updating parameter values and parameter covariance matrix elements, based on information contained in the data currently being analyzed. These formulae, in their several guises, are hereafter referred to as Bayes' equations. Derivation of Bayes' equations is given in Sect. II.A. Implementation of Bayes' equations in the code SAMMY is described in Sect. II.B.

II.A DERIVATION OF BAYES' EQUATIONS

A general outline of the derivation of Bayes' equations is given here. Algebraic details follow in Sect. II.A.1. The iteration scheme which compensates for non-linearity is discussed in Sect. II.A.2.

Bayes' theorem may be written in the form

$$p(P|DX) = p(P|X)\, p(D|PX) \tag{IIA.1}$$

where

1. P represents the parameters of the (extended) R-matrix theory and D represents the experimental data to be analyzed.
2. X represents "background" or "prior" information such as the data from which prior knowledge of the parameters P was derived. X is assumed to be independent of D.
3. $p(P|DX)$ is the probability for the value of the parameters, conditional upon the new data D, and is what we seek. It is conventional to call $p(P|DX)$ the posterior probability. Since P represents several parameters, $p(P|DX)$ is a joint probability density function (joint pdf.). The expectation values of P times $p(P|DX)$ are taken as the new estimates for the parameters; the associated covariance matrix gives us a measure of how well the parameters are determined and of the inter-dependencies of those determinations.
4. $p(D|PX)$ is the probability density function for observing the data D given that the parameters P are correct. It is a function of the parameters P of the model and is proportional to the likelihood function of the data D.
5. $p(P|X)$ is the joint pdf for the values of the parameters P of the model, prior to consideration of the new data D; it is known as the prior joint pdf. The expectation values of P times $p(P|X)$ are the prior estimates for the values of the parameters; the associated covariance matrix gives a measure of how well the parameters are known before consideration of the new data.

Let $P = \{P_k\}$ for $k = 1$ to K be the set of all parameters of the theoretical model to be considered. The joint pdf $p(P|X)$ is assumed to be a joint normal pdf having as expectation value the vector $\bar{P}$ and the covariance matrix M. Under this assumption the pdf may be written

$$p(P|X) \propto \exp\left[-\frac{1}{2} (P-\bar{P})^t\, M^{-1}\, (P-\bar{P}) \right] , \tag{IIA.2}$$

where the superscript t denotes the transpose.

The experimental data are represented by a data vector D whose components D_i are the L data points. The experimental conditions are assumed to be such that the data D (i.e., the D_i's) have a joint normal distribution with mean $T = T(P)$ and covariance matrix V. The likelihood function is then

$$p(D|PX) \propto \exp\left[-\frac{1}{2}(D-T)^t \, V^{-1} \, (D-T) \right] \quad . \tag{IIA.3}$$

Here T represents theory (i.e., calculated values of cross section or transmission), and the covariance matrix V represents not only the experimental "errors" of the data, but also any theoretical "errors" resulting from approximations used in calculating T. Obviously V need not be diagonal.

Combining Eqs. (IIA.1, .2, and .3) gives an expression for the pdf of P after consideration of new data D [i.e., for $p(P|DX)$], expressed in terms of the "true" value T. What is needed, however, is an expressions for $p(P|DX)$ expressed in terms of the parameters P. This is obtained formally by considering T a function of P, performing a Taylor expansion about $\bar{P}$ [the expectation value of $p(P|X)$], and keeping only the linear terms:

$$T(P) \cong \bar{T} + G(P-\bar{P}) \quad , \tag{IIA.4}$$

where $\bar{T}$ is equal to $T(\bar{P})$. The elements of G are the partial derivatives of T_n with respect to the parameters P_k, evaluated at $P = \bar{P}$:

$$G_{nk} = \left. \frac{\partial T_n}{\partial P_k} \right|_{P=\bar{P}} \qquad \text{for } n = 1 \text{ to } L \quad \text{and} \quad k = 1 \text{ to } K \tag{IIA.5}$$

Since T is a vector of dimension L (equal to the number of data points), and P is a vector of dimension K (equal to the number of parameters), this "sensitivity matrix" G is of dimension $L \times K$.

Substituting Eq. (IIA.4) into Eq. (IIA.3) and using Eq. (IIA.2), we obtain for the posterior joint pdf [Eq. (IIA.1)]

$$p(P|DX) \propto \exp\left[-\frac{1}{2} \left\{ (P-\bar{P})^t \, M^{-1} \, (P-\bar{P}) + \left(D-\bar{T}-G(P-\bar{P})\right)^t \, V^{-1} \left(D-\bar{T}-G(P-\bar{P})\right) \right\} \right] \quad . \tag{IIA.6}$$

Because of the three basic assumptions we have made, that is,

i. the prior joint pdf is a joint normal,

ii. the likelihood function is a joint normal,

iii. the true value is a linear function of the parameters,

it follows that the posterior joint pdf is also a joint normal. Denoting its expectation value by $\bar{P}'$ and its covariance matrix by M', we may write

$$p(P|DX) \propto \exp\left[-\frac{1}{2} \left\{ (P-\bar{P}')^t M'^{-1} (P-\bar{P}') \right\} \right] \qquad \text{(IIA.7)}$$

As shown in the next subsection, equating the linear and quadratic terms of the exponents in Eqs. (IIA.6) and (IIA.7) yields our final results, hereafter referred to as Bayes' equations:

$$P' - \bar{P} = MG^t (N+V)^{-1} (D-\bar{T}) \quad , \qquad \text{(IIA.8)}$$

and

$$M - M' = MG^t (N+V)^{-1} GM \quad , \qquad \text{(IIA.9)}$$

where the $L \times L$ matrix N is defined as

$$N = GMG^t \qquad \text{(IIA.10)}$$

The matrix N is the covariance matrix of the joint pdf for the true value of the data based upon our prior pdf for the value of the parameters. Since this form of Bayes' equations involves the inverse of ($N + V$), within SAMMY it is known as the "$N + V$ inversion scheme" or "NPV inversion scheme" (See Table VIA.2); this is the only form implemented in the earliest versions of SAMMY. For more algebraic details on this form, see [NL82].

An alternative form for Bayes' equations is the "$I + Q$ inversion scheme" (or "IPQ scheme"), which involves the inversion of a $K \times K$ non-symmetric matrix:

$$\bar{P}' - \bar{P} = M (I+Q)^{-1} G^t V^{-1} (D-\bar{T}) \quad , \qquad \text{(IIA.11)}$$

and

$$M' = M (I+Q)^{-1} \quad , \qquad \text{(IIA.12)}$$

where Q is defined as

$$Q = G^t V^{-1} GM \quad . \qquad \text{(IIA.13)}$$

A third form of Bayes' equations is the "$M+W$ inversion scheme" (or "MPW scheme"), which involves the inversion of a $K \times K$ symmetric matrix:

$$\bar{P}' - \bar{P} = M' G^t V^{-1} (D-\bar{T}) \quad , \qquad \text{(IIA.14)}$$

and

$$M' = (M^{-1} + W)^{-1} \quad , \tag{IIA.15}$$

where W is defined as

$$W = G^t V^{-1} G \quad . \tag{IIA.16}$$

The NPV inversion scheme is useful either when the data covariance matrix V contains off-diagonal elements, or when there are more varied parameters than there are data points (i.e., when $K > L$). (With Bayes' equations, as opposed to least squares, that situation is permissible.) For many situations in the resolved-resonance region, the IPQ and MPW schemes are more appropriate: There are more data points than varied parameters ($L > K$), and the data covariance matrix is either diagonal or of a form that can be readily inverted.

In the limit where the prior parameter covariance matrix M is diagonal and its elements tend to infinity, Bayes' equations becomes the familiar least-squares equations. This is most readily apparent in the MPW inversion scheme, which reduce to the least-squares equations by setting $M^{-1} = 0$ in Eq. (IIA.15).

Because the linearity condition of Eq. (IIA.4) may be only approximately correct, it is necessary to alter Bayes' equations slightly to permit iteration to an accurate solution. (Details are given in Sect. II.A.2.) It is the iterative form of Bayes' equations which is implemented in the SAMMY code.

Finally, we note that the derivation of Bayes' equations which we present in Sect. II.A.1 is not the only possible derivation. Alternatives can be found in [JM80] and [AG73].

II.A.1 Details of the Derivation

In Sect. II.A, we stated that Bayes' equations may be derived directly from Bayes' theorem,

$$p(P|DX) = p(P|X)\,p(D|PX) \quad , \tag{IIA1.1}$$

provided the three basic assumptions are met. These assumptions are:

i. the prior joint pdf is a joint normal. That is, the pdf for the parameters, prior to consideration of the data D, is

$$p(P|X) \propto \exp\left[-\frac{1}{2}(P-\bar{P})^t\, M^{-1}\, (P-\bar{P}) \right] \quad , \tag{IIA1.2}$$

ii. the likelihood function is a joint normal. That is, the pdf for the experimental data is

$$p(D|PX) \propto \exp\left[-\frac{1}{2}(D-T)^t\, V^{-1}\, (D-T) \right] \quad . \tag{IIA1.3}$$

iii. the true value is a linear function of the parameters. That is, a Taylor expansion of the theoretical values around the prior expectation values of the parameters truncates after the linear term,

$$T(P) \cong \bar{T} + G(P-\bar{P}) \quad , \tag{IIA1.4}$$

where the sensitivity matrix G is defined by

$$G_{ik} = \left. \frac{\partial T_i}{\partial P_k} \right|_{P=\bar{P}} \quad , \tag{IIA1.5}$$

and the theoretical value $\bar{T}_i$ (i.e., $\bar{T}$ for data point i) is also evaluated at $P = \bar{P}$.

Given these three assumptions, the posterior pdf $p(P|DX)$ is also a joint normal distribution and may be written

$$p(P|DX) \propto \exp\left[-\frac{1}{2}\left\{ (P-\bar{P}')^t\, M'^{-1}\, (P-\bar{P}') \right\} \right] \tag{IIA1.6}$$

Substituting Eq. (IIA1.2) through (IIA1.6) into Eq. (IIA1.1) and equating the exponents yield, in matrix form,

$$(P-\bar{P}')^t\, M'^{-1}\, (P-\bar{P}') + Y = (P-\bar{P})^t\, M^{-1}\, (P-\bar{P}) + \left(D-\bar{T}-G(P-\bar{P})\right)^t\, V^{-1}\, \left(D-\bar{T}-G(P-\bar{P})\right) \quad , \tag{IIA1.7}$$

where Y represents the normalization constant and is independent of P. Setting $P - \bar{P} = P - \bar{P}' + \bar{P}' - \bar{P}$ in Eq. (IIA1.7), and rearranging terms, we obtain

$$
\begin{aligned}
&(P-\bar{P}')^t\, M'^{-1}\, (P-\bar{P}') + Y \\
&\quad = (P-\bar{P}')^t \left(M^{-1} + G^t V^{-1} G\right)(P-\bar{P}') \\
&\quad + (P-\bar{P}')^t \left[\left(M^{-1} + G^t V^{-1} G\right)(\bar{P}'-\bar{P}) - G^t V^{-1}(D-\bar{T})\right] \\
&\quad + \left[(\bar{P}'-\bar{P})^t \left(M^{-1} + G^t V^{-1} G\right) - (D-\bar{T})^t V^{-1} G\right](P-\bar{P}') \\
&\quad + (\bar{P}'-\bar{P})^t\, M^{-1}\, (\bar{P}'-\bar{P}) + \left(D-\bar{T}-G(\bar{P}'-\bar{P})\right)^t V^{-1} \left(D-\bar{T}-G(\bar{P}'-\bar{P})\right) .
\end{aligned}
\tag{IIA1.8}
$$

Because Eq. (IIA1.8) must hold for all values of P, we may equate terms quadratic, linear, or constant in $(P-\bar{P}')$. From the quadratic we obtain Bayes' equation for updating the covariance matrix, and from the linear we obtain Bayes' equation for updating parameter values. The constant yields the invariant "Bayesian χ^2".

We begin with the covariance matrix; the coefficients of the quadratic $(P-\bar{P}')^t \ldots (P-\bar{P}')$ in Eq. (IIA1.8) yield

$$(M')^{-1} = M^{-1} + G^t V^{-1} G \quad , \tag{IIA1.9}$$

which is the form used in the MPW inversion scheme, with $W = G^t V^{-1} G$. Algebraic manipulation of this matrix equation gives us the form used in the other inversion schemes:

$$(M')^{-1} M = M^{-1} M + G^t V^{-1} G M = I + G^t V^{-1} G M \quad ,$$

where I represents the identity matrix. Multiplying by M' gives

$$M' (M')^{-1} M = M' + M' G^t V^{-1} G M \quad ,$$

which reduces to

$$M = M' (I + G^t V^{-1} G M) \quad , \tag{IIA1.10}$$

Thus we may define Q as

$$Q = G^t V^{-1} G M \quad , \tag{IIA1.11}$$

(as in Eq. (IIA.13) and obtain from Eq. (IIA1.10) the result

$$M' = M (I + G^t V^{-1} G M)^{-1} \quad , \tag{IIA1.12}$$

which is exactly Bayes' equation for updating the covariance matrix in the IPQ inversion scheme, Eq. (IIA.12).

To obtain the NPV version of Bayes' equations for the covariance matrix, further algebraic manipulation is required. Using the identity

$$X^{-1} = Z(XZ)^{-1} \tag{IIA1.13}$$

with

$$X = I + G^t V^{-1} G M = I + Q \tag{IIA1.14}$$

and

$$Z = G^t (N+V)^{-1} G \quad , \tag{IIA1.15}$$

where

$$N = GMG^t \quad , \tag{IIA1.16}$$

gives, from Eq. (IIA1.12),

$$\begin{aligned} M' &= MG^t (N+V)^{-1} G \left(\left(I + G^t V^{-1} G M \right) G^t (N+V)^{-1} G \right)^{-1} \\ &= MG^t (N+V)^{-1} G \left(G^t (N+V)^{-1} G + G^t V^{-1} G M G^t (N+V)^{-1} G \right)^{-1} . \end{aligned} \tag{IIA1.17}$$

Substituting the value for N and rearranging give

$$M' = MG^t (N+V)^{-1} G \left(G^t \left\{ (N+V)^{-1} + V^{-1} N (N+V)^{-1} \right\} G \right)^{-1} . \tag{IIA1.18}$$

The quantity in curly brackets is equal to V^{-1}; making that substitution and introducing the identity $V V^{-1} = I$ into the expression give

$$M' = MG^t (N+V)^{-1} V V^{-1} G \left(G^t V^{-1} G \right)^{-1} . \tag{IIA1.19}$$

Replacing V by its equivalent $N + V - N$ then gives

$$\begin{aligned} M' &= MG^t (N+V)^{-1} (N+V-N) V^{-1} G \left(G^t V^{-1} G \right)^{-1} \\ &= MG^t V^{-1} G \left(G^t V^{-1} G \right)^{-1} - MG^t (N+V)^{-1} N V^{-1} G \left(G^t V^{-1} G \right)^{-1} . \end{aligned} \tag{IIA1.20}$$

When N is replaced by its definition in the second of these terms, the equation immediately collapses to the form

$$M' = M - MG^t (N+V)^{-1} G M \quad , \tag{IIA1.21}$$

which is exactly the NPV version of Bayes' equation for updating the covariance matrix, Eq. (IIA.9).

If the indices for the matrices in EQ. (IIA1.21) are explicitly displayed, the equation becomes

$$M'_{kl} = M_{kl} - \sum_{n=1}^{K} \sum_{i=1}^{L} \sum_{j=1}^{L} \sum_{m=1}^{K} M_{kn} G_{in} \left((N+V)^{-1} \right)_{ij} G_{jm} M_{ml} \quad , \qquad \text{(IIA1.22)}$$

where N is given by

$$N_{ij} = \sum_{n=1}^{K} \sum_{m=1}^{K} G_{in} M_{nm} G_{jm} \quad . \qquad \text{(IIA1.23)}$$

To obtain Bayes' equation for updating the parameter values, we equate the linear terms of Eq. (IIA1.8). Since the left-hand-side of that equation has no terms linear in $(P - \bar{P}')$, the coefficient of $(P - \bar{P}')$ on the right-hand side must be zero. That is,

$$\left(M^{-1} + G^t V^{-1} G \right) (\bar{P}' - \bar{P}) = G^t V^{-1} (D - \bar{T}) \quad . \qquad \text{(IIA1.24)}$$

From Eq. (IIA1.9), the first quantity on the left is just M'^{-1}; we therefore have

$$\bar{P}' - \bar{P} = M' G^t V^{-1} (D - \bar{T}) \quad , \qquad \text{(IIA1.25)}$$

which is the form that Bayes' equation takes in the MPW inversion scheme, Eqs. (IIA.14). Substituting for M' from Eq. (IIA1.12) gives the form used in the IPQ inversion scheme,

$$\bar{P}' - \bar{P} = M(I+Q)^{-1} G^t V^{-1} (D - \bar{T}) \quad , \qquad \text{(IIA1.26)}$$

as in Eq. (IIA.11).

To obtain the expression needed for the NPV inversion scheme, replace M' in Eq. (IIA1.25) with Eq. (IIA1.22) to give

$$\bar{P}' - \bar{P} = \left(M - M G^t (N+V)^{-1} G M \right) G^t V^{-1} (D - \bar{T}) \quad , \qquad \text{(IIA1.27)}$$

which reduces to

$$\bar{P}' - \bar{P} = M G^t (N+V)^{-1} (D - \bar{T}) \quad . \qquad \text{(IIA1.28)}$$

Explicitly displaying the indices in this equation gives

$$\bar{P}_k' - \bar{P}_k = \sum_{l=1}^{K} \sum_{i=1}^{L} \sum_{j=1}^{L} M_{kl} G_{il} \left((N+V)^{-1} \right)_{ij} (D_j - \bar{T}_j) \quad . \qquad \text{(IIA1.29)}$$

Finally, we note that the constant term in Eq. (IIA1.8) may be simplified using Eq. (IIA1.29) to give

$$Y = (D-\overline{T})^t \left[(N+V)^{-1} GMG^t (N+V)^{-1} + (I-(N+V)^{-1}N)\, V^{-1} (I-N(N+V)^{-1})\right](D-\overline{T}) \quad , \tag{IIA1.30}$$

which reduces to

$$Y = (D-\overline{T})^t (N+V)^{-1} (D-\overline{T}) \tag{IIA1.31}$$

In SAMMY, this quantity is referred to as the "Bayesian χ^2". In the IPQ inversion scheme, this quantity can be simplified to the form

$$Y = (D-\overline{T})^t V^{-1} (D-\overline{T}) - (D-\overline{T})^t V^{-1} GM(I+Q)^{-1} G^t V^{-1} (D-\overline{T}) \tag{IIA1.32}$$

in which the first term is the usual (least-squares) χ^2, and the second term can be viewed as a "correction" to χ^2. The Bayesian χ^2 is, in some sense, a measure of the "best fit" than can be found between this theoretical formulation and these experimental data. The goal of a Bayes fit is, essentially, to have the value of the least-squares χ^2 become as near as possible to the value of the Bayesian χ^2 .

II.A.1.a Implicit data covariance matrix

Bayes' Equations, as derived above, can be modified slightly to efficiently incorporate certain types of off-diagonal data covariance matrices. Often (e.g., in the case of normalization or background subtraction) it is possible to write the data covariance matrix as the sum of two terms, the first of which is diagonal and the second of which is "separable" in the sense that

$$V^{ij} = v^i \delta_{ij} + \sum_k X_k^i w_k X_k^j \qquad \text{(IIA1 a.1)}$$

In this case the modification to the (N+V) version of Bayes' equations is immediate: simply replace V by $v + XwX^t$. The modification to the (I+Q) version is not so obvious, but may be far more important because it eliminates the need for inversion of a very large matrix. Note that V can be inverted via

$$V^{-1} = (v + XwX^t)^{-1} = v^{-1} - v^{-1}X(w^{-1} + X^t v^{-1} X)^{-1} X^t v^{-1} \quad . \qquad \text{(IIA1 a.2)}$$

Although it appears far messier to calculate this than to invert $v + XwX^t$ directly, in practice this is the easier calculation, because the dimension of w is small (~ 10's) while the dimension of v can be very large (~1000's). Substituting Eq. (IIA1a.2) into (IIA1.11) or (IIA.13) gives

$$Q = G^t v^{-1} GM - G^t v^{-1} X(w^{-1} + X^t v^{-1} X)^{-1} X^t v^{-1} GM \quad , \qquad \text{(IIA1 a.3)}$$

which is then used directly to calculate M' and P' in Eqs. (IIA.11) and (IIIA.12).

In SAMMY, implicit data covariance matrices can be used for normalization and background correction factors. Please see Section VI.C.3 for details.

II.A.2 Iteration Scheme

The linearity hypothesis, i.e., the assumption that the Taylor expansion of the theoretical values around the prior expectation value truncates after the linear term, is in general only approximately true. Therefore, the parameter values $\bar{P}'$ resulting from application of Bayes' equations are also only approximately correct. To obtain more accurate values, the Taylor expansion, Eq. (IIA1.4), may be performed not around $\bar{P}$ but around the new (intermediate) values $\bar{P}^{(n)}$, where n represents the nth iteration and $\bar{P}^{(0)} = \bar{P}$. That is, we assume

$$T \approx \bar{T}^{(n)} + G^{(n)} (P - \bar{P}^{(n)}) \quad . \tag{IIA2.1}$$

Here the sensitivity matrix $G^{(n)}$ and the theoretical values $\bar{T}^{(n)}$ are evaluated at $P = \bar{P}^{(n)}$. With EQ. (IIA2.1) for T, the formula analogous to Eq. (IIA1.7) is

$$\begin{aligned} &(P - \bar{P}^{(n+1)})^t \, M'^{-1} \, (P - \bar{P}^{(n+1)}) + Y \\ &= (P - \bar{P}^{(n)})^t \, M^{-1} \, (P - \bar{P}^{(n)}) \\ &\quad + \left(D - \bar{T}^{(n)} - G^{(n)} (P - \bar{P}^{(n)})\right)^t \, V^{-1} \left(D - \bar{T}^{(n)} - G^{(n)} (P - \bar{P}^{(n)})\right) \quad . \end{aligned} \tag{IIA2.2}$$

Setting P equal to $P - \bar{P}^{(n+1)} + \bar{P}^{(n+1)}$ everywhere in the right-hand side of Eq. (IIA2.2) gives the formula analogous to Eq. (IIA1.8) with $\bar{T}$ in that expression replaced by $\bar{T}^{(n)} + G^{(n)} (\bar{P} - \bar{P}^{(n)})$ and G by $G^{(n)}$. The iterative forms of Bayes' equations follow immediately.

For the NPV inversion scheme, the equations take the form

$$P' - \bar{P}^{(n+1)} = M G^{(n)t} \, (N^{(n)} + V)^{-1} \left(D - T^{(n)} - G^{(n)} (\bar{P} - \bar{P}^{(n)})\right) \quad , \tag{IIA2.3}$$

$$M - M^{(n+1)} = M G^{(n)t} \, (N^{(n)} + V)^{-1} \, G^{(n)} M \quad , \tag{IIA2.4}$$

while $N^{(n)}$ is defined as

$$N^{(n)} = G^{(n)} M G^{(n)t} \quad . \tag{IIA2.5}$$

For the IPQ inversion scheme, the iterative forms of Bayes' equations are

$$\bar{P}^{(n+1)} - \bar{P} = M\,(I+Q^{(n)})^{-1}\,G^{(n)t}\,V^{-1}\left(D-\bar{T}^{(n)}-G^{(n)}(\bar{P}-P^{(n)})\right)\,, \qquad \text{(IIA2.6)}$$

$$M^{(n+1)} = M\,(I+Q^{(n)})^{-1}\,, \qquad \text{(IIA2.7)}$$

where $Q^{(n)}$ is given by

$$Q^{(n)} = G^{(n)t}\,V^{-1}\,G^{(n)}\,M\,. \qquad \text{(IIA2.8)}$$

For the MPW inversion scheme, the iterative forms are

$$\bar{P}^{(n+1)} - \bar{P} = M^{(n+1)}\,G^{(n)t}\,V^{-1}\left(D-\bar{T}^{(n)}-G^{(n)}(\bar{P}-\bar{P}^{(n)})\right)\,, \qquad \text{(IIA2.9)}$$

with

$$M^{(n+1)} = (M^{-1}+W^{(n)})^{-1}\,, \qquad \text{(IIA2.10)}$$

and

$$W^{(n)} = G^{(n)t}\,V^{-1}\,G^{(n)}\,. \qquad \text{(IIA2.11)}$$

II.B IMPLEMENTATION OF BAYES' EQUATIONS

SAMMY's method of solution of Bayes' equations for NPV inversion scheme is described in Sect. II.B.1, and the solution for the IPQ scheme in Sect. II.B.2. The MPW solution method is discussed in Sect. II.B.3.

See Section II.C for a description of the various types of parameters which can be adjusted (varied, fitted via Bayes' equations) to fit the experimental data.

II.B.1 Solving Bayes' equations: (N + V) inversion scheme

SAMMY uses an early version of the code BAYES [NL82] to solve Bayes' equations in the (N + V) inversion scheme. In matrix notation, the non-iterative form of Bayes' equations can be written

$$\bar{P}' - \bar{P} = M G^t (N+V)^{-1} (D - \bar{T}) \quad , \tag{IIB1.1}$$

and

$$M' = M - MG^t (N+V)^{-1} GM \quad , \tag{IIB1.2}$$

where N is given by

$$N = GMG^t \quad . \tag{IIB1.3}$$

Solving these equations is equivalent to solving

$$AX = Y \tag{IIB1.4}$$

$K + 1$ times (where K is the number of parameters for the problem), with A the $L \times L$ symmetric matrix $N + V$ (where L is the number of data points), and Y a column matrix equal to $(D - \bar{T})$ in Eq. (IIB1.1) or equal to each of the K columns of the rectangular matrix GM in Eq. (IIB1.2).

The inverse of matrix A is not evaluated directly. Rather, A is first factorized as

$$A = UBU^t \tag{IIB1.5}$$

where B is a block-diagonal matrix, and U is the product of elementary unit triangular and permutation matrices, so that inverses of U and B are immediately available. The solution X to Eq. (IIB1.4) is then found from

$$X = (U^{-1})^t B^{-1} U^{-1} Y \quad . \tag{IIB1.6}$$

In SAMMY, the factorization of Eq. (IIB1.5) is performed by the LINPACK [JD79] subroutine SSPCO, and the $(K + 1)$ solutions are obtained by LINPACK subroutine SSPSL (with the author's updates for double precision). Subroutine NEWPAR oversees these operations.

It is necessary to modify this procedure slightly to account for the approximations built into Bayes' equations. As explained in Sec. IIA.2, an iteration scheme has been derived to correct for the non-linear relationship between parameters and theoretical values. The default in SAMMY is to preform two iterations, since (1) further iteration is expected to increase precision but not accuracy, and (2) test cases have shown this to yield consistent results. To reassure himself/herself that this is appropriate, the interested reader may refer to Example 4 of the original SAMMY manual [NL80], or make his/her own tests on his/her own data. Table VIA.1, Card Set 2, indicates the relevant parameter (ITMAX) to use. Note that k iterations (ITMAX = k) will yield the solution set $\bar{P}^{(k)}$ and $M^{(k)}$ from Eqs. (IIA2.3) and (IIA2.4).

Note to users of very early SAMMY version: The meaning of ITMAX has been changed from that in use prior to April 1984, and now corresponds exactly to the number of times that Bayes' equations are to be solved. Cavaet: The default value is ITMAX = 2; hence, putting zero (or blank) into column 50 of Card Set 2 of the INPut file will give ITMAX = 2, not ITMAX = 0. To obtain zero iterations (i.e., to evaluate the cross section but not update the parameter values), the user must specify "DO NOT SOLVE BAYES Equations" in the INPut file.

II.B.2 Solving Bayes' equations: (I + Q) inversion scheme

In matrix form, the non-iterative form of Bayes' equations for the (I + Q) inversion scheme can be written

$$\bar{P}' - \bar{P} = M\,(I+Q)^{-1} G^t V^{-1}\,(D-\bar{T}) \quad , \tag{IIB2.1}$$

and

$$M' = M\,(I+Q)^{-1} \quad , \tag{IIB2.2}$$

where Q is given by

$$Q = G^t V^{-1} G M \quad . \tag{IIB2.3}$$

Note that, although Q (and thus $I+Q$) is not symmetric, nevertheless M' is symmetric. This can be shown by noting that

$$M' = M(I+Q)^{-1} = M\left(M + MG^t V^{-1} G M\right)^{-1} M \tag{IIB2.4}$$

provided that M^{-1} exists. In the form of Eq. (IIB2.4), M' is clearly symmetric.

The inversion of $(I+Q)$ is found by using NAG [NAG] routine F01AAF. When M' is needed (i.e., for the final iteration), Eq. (IIB2.2) is solved first and the array M' used in Eq. (IIB2.1) to find $\bar{P}'$. When M' is not needed, the quantity $(I+Q)^{-1} G^t V^{-1}\,(D-\bar{T})$ is first generated and then the multiplication by M is performed. Fewer computer operations and thus faster run time result from performing the multiplications in this order.

As with the (N + V) inversion scheme, two iterations is the default in SAMMY.

The user has the option to choose which inversion scheme to use, or SAMMY can make the choice automatically. Generally, the (N + V) inversion scheme should be used unless the number of parameters is considerably smaller than the number of data points. If the data covariance matrix V is neither diagonal nor separable (see Sect. II.A.1.a), then the (N + V) inversion scheme **must** be used. When SAMMY is left to choose automatically, its choice will be the (N + V) inversion scheme unless both (1) V is diagonal or implicit, and (2) less array storage space is required for the (I + Q) scheme.

II.B.3 Solving Bayes' equations: (M + W) inversion scheme

The non-iterative form of Bayes' equations for the (M + W) inversion scheme can be written

$$\bar{P}' - \bar{P} = M' Y \quad , \tag{IIB3.1}$$

with Y defined as

$$Y = G^t V^{-1} (D - \bar{T}) \quad , \tag{IIB3.2}$$

and

$$M' = (M^{-1} + W)^{-1} \quad , \tag{IIB3.3}$$

where W is given by

$$W = G^t V^{-1} G \quad . \tag{IIB3.4}$$

The inverse of M is relatively easy to obtain. Initially M is generally diagonal, so the inverse is trivial. After the initial step, M is no longer diagonal but the inverse is already known from Eq. (IIB3.3) at the previous step.

The solution of Eqs. (IIIB3.1 through .4) is found from LINPACK [JD79] routines, in the same manner as the solution is found for the (N + V) inversion scheme.

The (M + W) inversion scheme is available for use in Version M5 of the SAMMY code only for specific applications (although in the future this will likely be the primary method). For calculations in the unresolved-resonance region, (M + W) is the method used. In the resolved-resonance region, the (M + W) scheme currently may be used in a limited fashion, first employed a means of retroactively producing an approximate covariance matrix for an existing set of resonance parameters.

Test case tr82 has an example of the procedure for retroactively producing an approximate covariance matrix. Essentially, what is done is the following:

(1) Run SAMMY for each independent data set, with the phrase

GENERATE Y AND W MATRICES

included in the INPut file. This causes SAMMY to produce and store the sub-matrices Y_i and W_i, defined by

$$Y_i = G_i^t V_i^{-1} (D_i - \bar{T}_i) \tag{IIB3.5}$$

and

$$W_i = G_i^t V_i^{-1} G_i \quad . \tag{IIB3.6}$$

in which the subscript i denotes the specific data set.

(2) Once Y_i and W_i are known for each set of experimental data, they can be summed over i, giving

$$Y = \sum_i Y_i \qquad \text{(IIB3.7)}$$

and

$$W = \sum_i W_i \quad . \qquad \text{(IIB3.8)}$$

These matrices are then used in Bayes' equations, Eq. (IIB3.1) and Eq. (IIB3.3) respectively, to solve for updated parameter values and covariance matrix; this is accomplished by a final SAMMY run in which the INPut file includes the phrase

READ Y AND W MATRICES

When it is a *retroactive* covariance matrix that is needed (for example, when covariance information is needed to augment an existing ENDF evaluation), SAMMY's output covariance matrix can be assumed to be associated with the initial parameter values (rather than with the output parameter values). The user must keep in mind, however, that this is an approximation; the validity of that approximation should be tested by studying differences between the two sets of parameter values. In test case tr82, "no Bayes" runs are performed for each of the experimental data sets, using the output parameter values, for comparison with the cross sections generated by the initial parameter set.

II.C CONSTRUCTING THE PARAMETER SET

Several distinct types of parameters may be varied (i.e., "searched on," in least-squares jargon) in SAMMY. Input values for all varied parameters are given in the PARameter file, Table VIB.1. The different types of parameters are listed below; note that the list is not necessarily all-inclusive.

- Resonance energies and widths: that is, the Reich-Moore R-matrix parameters as described in Sect. III.A.1.b (or the Breit-Wigner parameters as discussed in Sect. III.C). Values for energies and widths are provided via Card Set 1 of Table VIB.1.
- The matching radii (or channel radii) for the different spin groups and/or potential scattering vs penetrabilities and shift factors. Values for the matching radii are given in Card Set 7 of Table VIB.1.
- The seven parameters of the external R-function. These are described in Sect. III.A.1.a; values are input to the code as shown in Card Set 3 of Table VIB.1.
- Effective temperature for Doppler broadening, as described in Sect. IV.A.1 and IV.F. Input is in Card Set 4 of Table VIB.1.
- Resolution broadening parameters. For the original formulation (Gaussian and/or exponential) of resolution broadening, Sect. IV.A., input is in Card Set 4 of Table VIB.1. For the Oak Ridge Resolution Function of Sect. IV.E, input is in Card Set 9. For the RPI Resolution Function of Sect. IV.G, input is in Card Set 14.
- Normalization and background functions. See Sect. V.E.1 for description and Card Sets 6 and 13 for input details.
- Abundances for the various nuclides. See Card Set 10 of Table VIB.1.
- Sample thickness n. See Card Set 4.

For each parameter of each type, the user sets a flag which specifies whether that particular parameter is to be varied. SAMMY counts the number NPAR of varied parameters, and sets up an array U of dimension NPAR. The initial values $\underline{P}$ needed in Bayes' equations (see, e.g., Eq. (IIA2.3)) are stored in U. These values are not necessarily the same as those input in the PARameter file, but bear some functional relationship to the input form. For example, U will equal the reduced width amplitude $\gamma_{\lambda c}$ rather than the channel width $\Gamma_{\lambda c}$ (see Eq. (IIIA1b.2)). Details concerning conversion to the "u-parameters" are given in the sections relevant to the particular parameter.

Input uncertainties and correlations are likewise converted to represent the uncertainties and correlations on the u-parameters. Let p_i represent a physical parameter as input in the PARameter file, and let u_i be the related u-parameter. Since $u_i = u_i(p_i)$ is a precisely-specified functional relationship, we also know $\partial u_i / \partial p_i$. Therefore, assuming u_i is unrelated to other parameters, a small increment in u_i is related to an increment in p_i via $\delta u_i = (\partial u_i / \partial p_i)\, \delta p_i$. This relationship may then be used to convert from the covariance matrix for p to the covariance matrix for u; i.e.

$$M_{ij} = <\delta u_i \, \delta u_j> = \frac{\partial u_i}{\partial p_i} <\delta p_i \, \delta p_j> \frac{\partial u_j}{\partial p_j} \qquad \text{(IIC.1)}$$

where M is the covariance matrix needed for Bayes' equations, and $<\delta p_i \, \delta p_j>$ represents the "input" or initial covariance matrix.

III.A.1 Cross Section in Terms of R-Matrix

The angle-integrated cross sections from entrance channel c to exit channel c' with total angular momentum J is represented by $\sigma^J_{cc'}$. (The subscripts c and c' represent both the physical configuration and the quantum numbers; a detailed description of the channel, as used in SAMMY, is given in Subsection III.B.1.) This cross section is given in terms of the scattering matrix $U^J_{cc'}$ as

$$\sigma^J_{cc'} = \frac{\pi}{k_c^2} g_c \left| \delta_{cc'} - U^J_{cc'} \right|^2 \quad , \tag{IIIA1.1}$$

where k_c is the wave number associated with incident channel c (see Subsection III.B.4) and g_c is the spin statistical factor (see Subsection III.B.1).

The total cross section (sum over all exit channels) may be expressed as

$$\sigma^{total} = \frac{2\pi}{k^2} \sum_J g_J \sum_{\substack{c = incident \\ channel}} \left(1 - Re(U^J_{cc}) \right) \quad , \tag{IIIA1.2}$$

in which the spin statistical factor g_c is removed from the sum over c and renamed g_J, since it depends only on the (conserved) total angular momentum J [and on the spins of the two particles in the incident channel]; likewise, the wave number for all incident channels (assuming there are more than one) is the same.

The elastic (or scattering) cross section is

$$\sigma^{elastic} = \frac{\pi}{k^2} \sum_J g_J \sum_{\substack{c = incident \\ channel}} \left(1 - 2\,Re(U^J_{cc}) + \sum_{\substack{c' = incident \\ channel}} \left| U^J_{cc'} \right|^2 \right) \quad . \tag{IIIA1.3}$$

Note that the innermost summation includes only those exit channels c' which are also incident channels. Similarly, the reaction cross section is given by

$$\sigma^{reaction} = \frac{\pi}{k^2} \sum_J g_J \sum_{\substack{c = incident \\ channel}} \sum_{\substack{c' = exit \\ channel}} \left| U^J_{cc'} \right|^2 \quad , \tag{IIIA1.4}$$

where the exit channel summation includes all non-elastic channels (fission, inelastic, ...). Individual reactions (e.g. fission) would be found by including only the relevant channels in the sum over c' in (IIIA1.4); the current release of SAMMY requires all exit channels to be included in the sum in that equation; future releases of SAMMY will permit individual channels.

Because the Reich-Moore approximation treats capture channels differently from particle channels, the capture cross section must found by subtracting all other cross sections from the total,

$$\sigma^{capture} = \sigma^{total} - \sigma^{elastic} - \sigma^{reaction} \quad , \tag{IIIA1.5}$$

or

$$\sigma^{capture} = \frac{\pi}{k^2} \sum_J g_J \sum_{\substack{c = incident \\ channels}} \left(1 - \sum_{\substack{c' = any \\ channel}} |U^J_{cc'}|^2 \right) \quad . \tag{IIIA1.6}$$

The absorption cross section is defined as the sum of $\sigma^{reaction}$ and $\sigma^{capture}$.

The scattering matrix U can be written in terms of the matrix W as

$$U^J_{cc'} = \Omega_l \, W^J_{cc'} \, \Omega_{l'} \quad , \tag{IIIA1.7}$$

where l represents the orbital angular momentum (see Subsection III.B.1), and Ω is given by

$$\Omega_l = e^{-i\varphi_l} \quad . \tag{IIIA1.8}$$

Expressions for the potential scattering phase shifts φ_l are shown in Table IIIA1.1 for non-Coulomb channels, and in Section III.H (page 56u) for Coulomb channels.

The matrix W in Eq. (IIIA1.7) is related to the R-matrix via (in matrix notation with indices suppressed)

$$W = P^{1/2} (I - RL)^{-1} (I - RL^*) P^{-1/2} \tag{IIIA1.9}$$

where the quantity L in Eq. (IIIA1.9) is given by

$$L = (S - B) + iP \tag{IIIA1.10}$$

with P the penetrability, S the shift factor, and B the arbitrary boundary constant at the channel radius a_c (see Table IIIA1.1 for non-Coulomb and Section III.H for Coulomb). The quantity I in Eq. (IIIA1.9) represents the identity matrix.

SAMMY uses a modified form of Eq. (IIIA1.9) to evaluate W. Since S, B, and P are all real, L^* may be expressed as $L - 2iP$, which gives

$$\begin{aligned} W &= P^{1/2}(I-RL)^{-1}(I-RL+2iRP)\,P^{-1/2} \\ &= P^{1/2}(I-RL)^{-1}(I-RL)\,P^{-1/2} + P^{1/2}(I-RL)^{-1}2iRPP^{-1/2} \\ &= I + P^{1/2}(I-RL)^{-1}2i\{-(I-RL)L^{-1}+L^{-1}\}P^{1/2} \quad , \end{aligned} \tag{IIIA1.11}$$

where the quantity in curly brackets is equal to R. Further simplification gives

Table IIIA1.1. Penetrability (penetration factor) P, level shift factor S, and potential scattering phase shift φ for orbital angular momentum l, center of mass momentum k, and channel radius a_c, with $\rho = ka_c$.

l	P_l	S_l	φ_l
0	ρ	0	ρ
1	$\rho^3/(1+\rho^2)$	$-1/(1+\rho^2)$	$\rho - \tan^{-1}\rho$
2	$\rho^5/(9+3\rho^2+\rho^4)$	$-(18+3\rho^2)/(9+3\rho^2+\rho^4)$	$\rho - \tan^{-1}[3\rho/(3-\rho^2)]$
3	$\rho^7/(225+45\rho^2+6\rho^4+\rho^6)$	$-(675+90\rho^2+6\rho^4)/(225+45\rho^2+6\rho^4+\rho^6)$	$\rho - \tan^{-1}[\rho(15-\rho^2)/(15-6\rho^2)]$
4	$\rho^9/(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8)$	$-(44100+4725\rho^2+270\rho^4+10\rho^6)/(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8)$	$\rho - \tan^{-1}[\rho(105-10\rho^2)/(105-45\rho^2+\rho^4)]$
l	$\dfrac{\rho^2 P_{l-1}}{(l-S_{l-1})^2 + P_{l-1}^2}$	$\dfrac{\rho^2 (l-S_{l-1})}{(l-S_{l-1})^2 + P_{l-1}^2} - l$	$\varphi_{l-1} - \tan^{-1}\left(P_{l-1}/(l-S_{l-1})\right)$ or $B_l = (B_{l-1} + X_l)/(1 + B_{l-1}X_l)$ where $B_l = \tan^{-1}(\rho - \varphi_l)$ and $X_l = (P_{l-1})/(l-S_{l-1})$

$$W = I - 2iP^{1/2}L^{-1}P^{1/2} + 2iP^{1/2}(I-RL)^{-1}L^{-1}P^{1/2}$$
$$= I - 2iPL^{-1} + 2iP^{1/2}L^{-1}(L^{-1}-R)^{-1}L^{-1}P^{1/2} \quad , \qquad \text{(IIIA1.12)}$$

which is the form used directly in SAMMY. If subscripts are reinserted, this expression becomes

$$W_{cc'} = \delta_{cc'}(1-2iP_l L_l^{-1}) + 2i\sqrt{P_l}\,L_l^{-1}\left[(I-RL)^{-1}\right]_{cc'}L_{l'}^{-1}\sqrt{P_{l'}} \quad . \qquad \text{(IIIA1.13)}$$

Using these definitions of U and W, the elastic cross section can be written as

$$\sigma^{elastic} = \frac{\pi}{k^2}\sum_J g_J \sum_{inc\,c}\left\{1 - 2\cos 2\varphi_l\, Re\, W^J_{cc} - 2\sin 2\varphi_l\, Im\, W^J_{cc} + \sum_{inc\,c'}|W^J_{cc'}|^2\right\} \quad . \qquad \text{(IIIA1.14)}$$

Similarly, the reaction cross section becomes

$$\sigma^{reaction} = \frac{\pi}{k^2}\sum_J g_J \sum_{inc\,c}\sum_{exit\,c'}|W^J_{cc'}|^2 \quad , \qquad \text{(IIIA1.15)}$$

and the capture cross section is

$$\sigma^{capture} = \frac{\pi}{k^2}\sum_J g_J \sum_{inc\,c}\left(1 - \sum_{all\,c'}|W^J_{cc'}|^2\right) \quad . \qquad \text{(IIIA1.16)}$$

Finally, the total cross section may be written as the sum of the others, or

$$\sigma^{total} = \frac{2\pi}{k^2}\sum_J g_J \sum_{inc\,c}\left\{1 - \cos 2\varphi_l\, Re\, W^J_{cc} - \sin 2\varphi_l\, Im\, W^J_{cc}\right\} \quad . \qquad \text{(IIIA1.17)}$$

These equations can of course be expanded in terms of R using the formulae on page 28. The matrix R can, in turn, be expanded in terms of resonances (levels) and "external" functions. Within SAMMY, there are two formulations for the Reich-Moore approximation to the R-matrix; the first is discussed in Section III.A.1.b on page 33 and the second in Section III.D on page 56g. In addition, the user may wish to include a logarithmic approximation to the external R-matrix; that is described in Section III.A.1.a on page 31.

III.A.1.a Logarithmic parameterization of external R-function

The "external R-function" is one particular approximation for the contribution to the R-matrix within a specified region of energy, intended to mimic the effect of those resonances or bound states external to that region. (Another, more commonly used, approximation is the inclusion of "dummy" resonances whose positions are external to the energy region of interest. SAMMY users should be aware that the use of dummy resonances is the only option permitted by ENDF formats.)

The logarithmic parameterization as implemented in SAMMY is as follows:

$$R_c^{ext}(E) = \bar{R}_{con,c} + \bar{R}_{lin,c}\,E + \bar{R}_{q,c}\,E^2 - s_{lin,c}\,(E_c^{up} - E_c^{down}) - (s_{con,c} + s_{lin,c}) \ln\left[\frac{E_c^{up} - E}{E - E_c^{down}}\right] \quad \text{(IIIA1a.1)}$$

Any or all of the seven free parameters may be varied during a SAMMY analysis (see Table VI.B.1, Card Set 3, and alternative to Card Set 3). Note that R^{ext} is strictly real in this parameterization.

The u-parameters (that is, the parameters on which Bayes' equations will operate; see Sect. II.C) associated with the external R-function are given by

$$\begin{aligned}
u(E_c^{down}) &= E_c^{down} \\
u(E_c^{up}) &= E_c^{up} \\
u(\bar{R}_{con,c}) &= \bar{R}_{con,c} \\
u(\bar{R}_{lin,c}) &= \bar{R}_{lin,c} \\
u(\bar{R}_{q,c}) &= \bar{R}_{q,c} \\
u(s_{con,c}) &= \sqrt{s_{con,c}} \\
u(s_{lin,c}) &= s_{lin,c}
\end{aligned} \quad \text{(IIIA1a.2)}$$

III.A.2.a Derivatives with respect to R-matrix parameters

For resonance and R^{ext} parameters, the derivative of the cross section may be written as

$$\frac{\partial \sigma}{\partial u_i} = \sum_{\substack{\mu \le \nu \\ \omega \le \tau}} \frac{\partial R_{\mu\nu}}{\partial u_i} \frac{\partial W_{\omega\tau}}{\partial R_{\mu\nu}} \frac{\partial U_{\omega\tau}}{\partial W_{\omega\tau}} \frac{\partial \sigma}{\partial U_{\omega\tau}} \qquad \text{(IIIA2a.1)}$$

where the index J has been suppressed, since it is fixed for a given u. The restricted sums ($\mu \le \nu, \omega \le \tau$) result from the symmetry of R and W. Each term in this expression will be evaluated separately, starting with the right-most term.

The derivatives of cross section with respect to the real part of U can be expresses as

$$\frac{\partial \sigma}{\partial U^r} = \frac{\partial \sigma}{\partial U} \frac{\partial U}{\partial U^r} + \frac{\partial \sigma}{\partial U^*} \frac{\partial U^*}{\partial U^r} = \frac{\partial \sigma}{\partial U} + \frac{\partial \sigma}{\partial U^*} = 2\, Re\left[\frac{\partial \sigma}{\partial U}\right] , \qquad \text{(IIIA2a.2)}$$

where the asterisk implies complex conjugate, and U and U^* are treated as independent entities. Similarly the derivative with respect to the imaginary part of U is given by

$$\frac{\partial \sigma}{\partial U^i} = \frac{\partial \sigma}{\partial U} \frac{\partial U}{\partial U^i} + \frac{\partial \sigma}{\partial U^*} \frac{\partial U^*}{\partial U^i} = i\frac{\partial \sigma}{\partial U} - i\frac{\partial \sigma}{\partial U^*} = -2\, Im\left[\frac{\partial \sigma}{\partial U}\right] . \qquad \text{(IIIA2a.3)}$$

Values for the partial derivative of σ with respect to U are found from Eqs. (IIIA1.2 through IIIA1.5), which give

$$\frac{\partial \sigma^{total}}{\partial U_{\omega\tau}} = -\frac{\pi g}{k^2} \delta_{\omega\tau} , \qquad \text{(IIIA2a.4)}$$

$$\frac{\partial \sigma^{elastic}}{\partial U_{\omega\tau}} = -\frac{\pi g}{k^2} (\delta_{\omega\tau} - U^*_{\omega\tau}) , \qquad \text{(IIIA2a.5)}$$

$$\frac{\partial \sigma^{reaction}}{\partial U_{\omega\tau}} = \frac{\pi g}{k^2} U^*_{\omega\tau} , \qquad \text{(IIIA2a.6)}$$

and

$$\frac{\partial \sigma^{capture}}{\partial U_{\omega\tau}} = -\frac{\pi g}{k^2} U^*_{\omega\tau} . \qquad \text{(IIIA2a.7)}$$

Derivatives of a complex variable (such as U) with respect to another complex variable (such as W) may be generated directly, without separately considering the real and imaginary parts of each variable; this is demonstrated explicitly in Sect. III.B.5. Here, we make use of this result to evaluated $\partial U / \partial W$ and $\partial W / \partial R$:

Derivatives of $U_{\omega\tau}$ with respect to $W_{\mu\nu}$ are formed directly from Eq. (IIIA1.7), which may be expressed as

$$U_{\omega\tau} = \Omega_{\omega} W_{\omega\tau} \Omega_{\tau} \qquad \text{(IIIA2a.8)}$$

so that

$$\frac{\partial U_{\omega\tau}}{\partial W_{\omega\tau}} = \Omega_{\omega} \Omega_{\tau} \quad . \qquad \text{(IIIA2a.9)}$$

Derivatives of W with respect to R are formed from Eq. (IIIA1.12), which we rewrite as

$$W_{\omega\tau} = \delta_{\omega\tau} \left(1 - 2 i P_{\omega} L_{\omega}^{-1}\right) + 2 i \sqrt{P_{\omega}}\, L_{\omega}^{-1}\, Y_{\omega\tau}\, L_{\tau}^{-1} \sqrt{P_{\tau}} \qquad \text{(IIIA2a.10)}$$

where we have set

$$Y_{\omega\tau} = \left[\left(L^{-1} - R\right)^{-1}\right]_{\omega\tau} \quad . \qquad \text{(IIIA2a.11)}$$

In [NL80, Appendix A], we show that the derivative of Y with respect to R is given by

$$\frac{\partial Y_{\omega\tau}}{\partial R_{\mu\nu}} = Y_{\omega\mu} Y_{\nu\tau} + Y_{\omega\nu} Y_{\mu\tau} (1 - \delta_{\mu\nu}) \quad . \qquad \text{(IIIA2a.12)}$$

Substitution of this expression into the derivative of Eq. (IIIA2a.10) gives

$$\frac{\partial W_{\omega\tau}}{\partial R_{\mu\nu}} = 2 i \sqrt{P_{\omega}}\, L_{\omega}^{-1} \left[Y_{\omega\mu} Y_{\nu\tau} + Y_{\omega\nu} Y_{\mu\tau} (1 - \delta_{\mu\nu}) \right] L_{\tau}^{-1} \sqrt{P_{\tau}} \qquad \text{(IIIA2a.13)}$$

Derivatives of R with respect to u depend upon which particular u-parameter is being considered. Parameters of the external R-matrix, resonance parameters, and channel width are described in the next three subsections.

III.A.2.a.ii Resonance parameters

From Eq. (IIIA1b.1), the derivative of R with respect to the resonance u-parameters can be found as

$$\frac{\partial\, Re[R_{\mu\nu}]}{\partial \sqrt{E_\lambda}} = \left[2\,\gamma_{\lambda\mu}\,\gamma_{\lambda\nu}\sqrt{E_\lambda}\,\right]\left[\frac{\left\{-(E_\lambda - E)^2 + (\alpha_\lambda^2)^2\right\}}{D_\lambda^2}\right], \qquad \text{(IIIA2aii.1)}$$

$$\frac{\partial\, Im[R_{\mu\nu}]}{\partial \sqrt{E_\lambda}} = \left[-4\,\gamma_{\lambda\mu}\,\gamma_{\lambda\nu}\sqrt{E_\lambda}\,\right]\left[\frac{\left\{-(E_\lambda - E)^2\ \alpha_\lambda^2\right\}}{D_\lambda^2}\right], \qquad \text{(IIIA2aii.2)}$$

$$\frac{\partial\, Re[R_{\mu\nu}]}{\partial\, \alpha_\lambda} = \left[-4\,\gamma_{\lambda\mu}\,\gamma_{\lambda\nu}\,\alpha_\lambda\,\right]\left[\frac{\left\{-(E_\lambda - E)^2\ \alpha_\lambda^2\right\}}{D_\lambda^2}\right], \qquad \text{(IIIA2aii.3)}$$

$$\frac{\partial\, Im[R_{\mu\nu}]}{\partial\, \alpha_\lambda} = \left[2\,\gamma_{\lambda\mu}\,\gamma_{\lambda\nu}\,\alpha_\lambda\,\right]\left[\frac{\left\{(E_\lambda - E)^2 - (\alpha_\lambda^2)^2\right\}}{D_\lambda^2}\right], \qquad \text{(IIIA2aii.4)}$$

$$\frac{\partial\, Re[R_{\mu\nu}]}{\partial\, \gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}(1+\delta_{\mu\nu})\right]\left[\frac{(E_\lambda - E)}{D_\lambda}\right], \qquad \text{(IIIA2aii.5)}$$

and

$$\frac{\partial\, Im[R_{\mu\nu}]}{\partial\, \gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}(1+\delta_{\mu\nu})\right]\left[\frac{\alpha_\lambda^2}{D_\lambda}\right], \qquad \text{(IIIA2aii.6)}$$

where

$$D_\lambda = (E_\lambda - E) + \alpha_\lambda^4 \ . \qquad \text{(IIIA2aii.7)}$$

In each of these equations, the first square bracket contains an energy-independent factor; in the code SAMMY, this factor is evaluated outside the energy-loop in subroutine BABB and is stored as BR(i,μν) for the derivative of the real part of $R_{\mu\nu}$ with respect to the i^{th} parameter, and BI(i,μν) for the derivative of the imaginary part of $R_{\mu\nu}$. The quantity in the second square bracket is energy-dependent but channel-independent. Therefore, it must be generated for each energy and is temporarily stored as UPR(i) and UPI(i) in subroutine ABPART.

To avoid problems arising from the computer's limited precision, and to minimize computing time, partial derivatives for non-s-wave resonances are truncated to zero far away from the resonance. The working definition of "far away" is 20 times the sum of the partial widths for that resonance, plus 3 times the sum of the Doppler and resolution-broadening widths, i.e. far beyond the region where a resonance can produce any noticeable effect. That is, the derivative of the cross section at energy E is set to zero for resonance level λ, if

$$|E - E_\lambda| > 20\left[\sum_c \Gamma_{\lambda c} + \Gamma_\lambda^\gamma\right] + 3(d+r) \qquad \text{(IIIA2aii.8)}$$

for resonances with $\ell > 0$, where d represents the Doppler and r the resolution width. Moreover, the contribution to the imaginary part of R is set to zero whenever the distance from level λ is greater than 100 times that specified in Eq. (IIIA2aii.8). (The contribution to the *real* part of R is never assumed negligible.)

For s-wave resonances ($\ell = 0$), the user has the option of setting derivatives equal to zero beyond a certain distance, where the distance is twice that specified for non-s-waves. (See Table VIA.2 for details on invoking this option.)

III.A.2.b Derivatives with respect to matching radius

Derivatives with respect to matching radius a require modification of the procedure outlined in Sect. III.A.2.a, since phase shifts φ and penetrabilities P also depend on matching radius. All dependence on a is via ρ, where

$$\rho = k a \quad , \tag{IIIA2b.1}$$

and k is described in Sect. III.B.4. Thus, we may write

$$\frac{\partial \sigma}{\partial a} = \frac{\partial \sigma}{\partial \rho}\frac{\partial \rho}{\partial a} = k\frac{\partial \sigma}{\partial \rho} \quad . \tag{IIIA2b.2}$$

Our problem therefore reduces to finding $\partial\sigma/\partial\rho$.

The derivative of the cross section with respect to ρ may be formed from Eq. (IIIA1.1),

$$\begin{aligned}\frac{\partial \sigma^J_{cc'}}{\partial \rho} &= \frac{\pi}{k_c^2} g_c^J \left[\left(\delta_{cc'} - U^J_{cc'}\right)\frac{\partial U^{J*}_{cc'}}{\partial \rho} + \left(\delta_{cc'} - U^{J*}_{cc'}\right)\frac{\partial U^J_{cc'}}{\partial \rho}\right] \\ &= \frac{2\pi}{k_c^2} g_c^J \left[\delta_{cc'}\frac{\partial Re(U^J_{cc'})}{\partial \rho} - Re\left(U^{J*}_{cc'}\frac{\partial U^J_{cc'}}{\partial \rho}\right)\right] .\end{aligned} \tag{IIIA2b.3}$$

From the definitions of Ω and φ, Eqs. (IIIA1.7, .8), the partial of U with respect to ρ may be written as

$$\frac{\partial U^J_{cc'}}{\partial \rho} = -i\frac{\partial \varphi_l}{\partial \rho} U^J_{cc'} + \Omega_l \frac{\partial W^J_{cc'}}{\partial \rho}\Omega_{l'} - i U^J_{cc'}\frac{\partial \varphi_{l'}}{\partial \rho} \quad , \tag{IIIA2b.4}$$

so that Eq. (IIIA2b.3) can be written

$$\begin{aligned}\frac{\partial \sigma^J_{cc'}}{\partial \rho} = \frac{2\pi}{k_c^2} g_c^J \Bigg\{ &\delta_{cc'} Re\left(-2i\frac{\partial \varphi_l}{\partial \rho} U^J_{cc} + \Omega_l^2 \frac{\partial W^J_{cc}}{\partial \rho}\right) \\ &- Re\left(U^{J*}_{cc'}\left[-i\left(\frac{\partial \varphi_l}{\partial \rho} + \frac{\partial \varphi_{l'}}{\partial \rho}\right) U^J_{cc'} + \Omega_l \frac{\partial W^J_{cc'}}{\partial \rho}\Omega_{l'}\right]\right)\Bigg\} \quad ,\end{aligned} \tag{IIIA2b.5}$$

or, since $\Omega_l \Omega^*_l = 1$,

$$\begin{aligned}\frac{\partial \sigma^J_{cc'}}{\partial \rho} = \frac{2\pi}{k_c^2} g_c^J Re\Bigg\{ &\delta_{cc'}\Omega_l^2 \left(-2i\frac{\partial \varphi_l}{\partial \rho} W^J_{cc} + \frac{\partial W^J_{cc}}{\partial \rho}\right) \\ &- \left(W^{J*}_{cc'}\left[-i\left(\frac{\partial \varphi_l}{\partial \rho} + \frac{\partial \varphi_{l'}}{\partial \rho}\right) W^J_{cc'} + \frac{\partial W^J_{cc'}}{\partial \rho}\right]\right)\Bigg\} .\end{aligned} \tag{IIIA2b.6}$$

Derivatives of hard sphere phase shifts φ are formed by direct differentiation of the formulae in Table IIIA1.1 for non-Coulomb and of the equations in Section III.H for Coulomb.

The derivatives of W are formed from Eq. (IIIA1.12):

$$\begin{aligned}\frac{\partial W^J_{cc'}}{\partial \rho} &= -2i\,\delta_{cc'}\,L_l^{-1}\,\frac{\partial P_l}{\partial \rho} + 2i\,\delta_{cc'}\,P_l\,L_l^{-2}\left(\frac{\partial S_l}{\partial \rho}+i\frac{\partial P_l}{\partial \rho}\right)\\ &+ 2i\,\frac{\partial P_l}{\partial \rho}\,\frac{1}{2\sqrt{P_l}}\,L_l^{-1}\,[(L^{-1}-R)^{-1}]_{cc'}\,L_{l'}^{-1}\,\sqrt{P_{l'}}\\ &+ 2i\,\sqrt{P_l}\,(-L_l^{-2})\left(\frac{\partial S_l}{\partial \rho}+i\frac{\partial P_l}{\partial \rho}\right)[(L^{-1}-R)^{-1}]_{cc'}\,L_{l'}^{-1}\,\sqrt{P_{l'}}\\ &+ 2i\,\sqrt{P_l}\,L_l^{-1}\,[(L^{-1}-R)^{-1}]_{cc'}\,(-L_{l'}^{-2})\left(\frac{\partial S_{l'}}{\partial \rho}+i\frac{\partial P_{l'}}{\partial \rho}\right)\sqrt{P_{l'}}\\ &+ 2i\,\sqrt{P_l}\,L_l^{-1}\,[(L^{-1}-R)^{-1}]_{cc'}\,L_{l'}^{-1}\,\frac{1}{2\sqrt{P_{l'}}}\,\frac{\partial P_{l'}}{\partial \rho}\\ &+ 2i\sum_{c''}\sqrt{P_l}\,L^{-1}\,[(L^{-1}-R)^{-1}]_{cc''}\,L_{l''}^{-1}\left(\frac{\partial S_{l''}}{\partial \rho}+i\frac{\partial P_{l''}}{\partial \rho}\right)L_{l''}^{-1}\,[(L^{-1}-R)^{-1}]_{c''c'}\,L_{l'}^{-1}\sqrt{P_{l'}}\end{aligned} \qquad \text{(IIIA2b.7)}$$

This expression can be greatly simplified by setting

$$X_{cc'} = \sqrt{P_l}\,L_l^{-1}\,[(L^{-1}-R)^{-1}]_{cc'}\,L_{l'}^{-1}\,\sqrt{P_{l'}} - P_l\,L_l^{-1}\,\delta_{ll'}\ , \qquad \text{(IIIA2b.8)}$$

which gives

$$\begin{aligned}\frac{\partial W^J_{cc'}}{\partial \rho} &= +i\,\frac{\partial P_l}{\partial \rho}\,\frac{1}{P_l}\,X_{cc'} + i\,X_{cc'}\,\frac{1}{P_{l'}}\,\frac{\partial P_{l'}}{\partial \rho}\\ &+ 2i\sum_{c''}X_{cc''}\,P_{l''}^{-1}\left(\frac{\partial S_{l''}}{\partial \rho}+i\frac{\partial P_{l''}}{\partial \rho}\right)X_{c''c'}\ .\end{aligned} \qquad \text{(IIIA2b.9)}$$

Derivatives of penetrabilities P_l and shift factors S_l are found by direct differentiation of the formulae in Table IIIA1.1 for non-Coulomb and Section III.H for Coulomb. Derivatives of the cross sections with respect to ρ are then found by substituting results from Eq. (IIIA2b.9) into Eq. (IIIA2b.6).

Prior to Release M5 of the code (Revision 5 of this users' guide), SAMMY did not have a reasonable treatment of non-varied neutron widths Γ_n when the corresponding radius was varied. Originally, it was the reduced width amplitude γ_n which was held fixed; hence, treating the radius as a search parameter resulted in changes in the unvaried neutron widths Γ_n (as printed in the output PARameter file, e.g.). Release M2 (and M2a) of the code included an option to hold the Γ_n's fixed (i.e., vary the γ_n's), but derivatives were not calculated in a totally consistent fashion. For the current release (M5 and subsequent), unvaried Γ_n are assumed to be constant; derivatives are (properly) calculated accordingly.

III.B.3 Evaluation of Hard-Sphere Phase Shift

Formulae for the hard-sphere phase shift (otherwise known as the potential scattering phase shift) are given in Table IIIA.1 for non-Coulomb interactions. What is actually needed in SAMMY is not, however, the phase shifts φ themselves, but rather $\cos(2\varphi)$ and $\sin(2\varphi)$. Since evaluation of φ requires the inverse tangent function, results for $\cos(2\varphi)$ and $\sin(2\varphi)$ are more readily generated with fewer computer roundoff errors by using trigonometric relationships to generate formulae for $\cos(2\varphi)$ and $\sin(2\varphi)$ directly.

Note from the table that, for all l, φ may be written in the form

$$\varphi = A - X \tag{IIIB3.1}$$

where

$$X = \tan^{-1} B \quad . \tag{IIIB3.2}$$

From Eq. (IIIB3.1) with elementary trigonometric relationships we find

$$\cos\varphi = \cos A \cos X + \sin A \sin X \tag{IIIB3.3}$$

and

$$\sin\varphi = -\cos A \sin X + \sin A \cos X \quad . \tag{IIIB3.4}$$

Thus, $\cos(2\varphi)$ becomes

$$\begin{aligned} \cos(2\varphi) &= 2\cos^2\varphi - 1 = 2\cos^2 A \cos^2 X (1 + \tan A \tan X)^2 - 1 \\ &= 2\frac{\cos^2 A}{1 + B^2}(1 + B\tan A)^2 - 1 \quad . \end{aligned} \tag{IIIB3.5}$$

Similarly, $\sin(2\varphi)$ can be written

$$\begin{aligned} \sin(2\varphi) &= 2\cos\varphi \sin\varphi = 2\cos^2 A \cos^2 X (1 + \tan A \tan X)(-\tan X + \tan A) \\ &= 2\frac{\cos^2 A}{1 + B^2}(1 + B\tan A)(-B + \tan A) \quad . \end{aligned} \tag{IIIB3.6}$$

Equations (IIIB3.5) and (IIIB3.6) are the form used in SAMMY to evaluate the hard-sphere phase shift terms.

III.B.4 Momentum in the Center of Mass System

The center-of-mass (com) momentum k needed in the formulae for cross sections (see Sect. III.A) may be found in terms of laboratory energy E by utilizing conservation of energy and momentum. Let p represent the momentum of the incident particle in the laboratory. Then the laboratory kinetic energy E is given by

$$E = p^2 / 2m_2 \quad , \tag{IIIB4.1}$$

or

$$p = \sqrt{2m_2 E} \quad , \tag{IIIB4.2}$$

where m_2 is the mass of the incident particle. If k is the neutron momentum (or, equivalently, the momentum of the sample nuclide, whose mass is m_1) in the center of mass system, then the energy *in* the com is

$$E_{\text{in com}} = k^2 / 2m_1 + k^2 / 2m_2 \quad . \tag{IIIB4.3}$$

The energy *of* the com is given by

$$E_{\text{of com}} = p^2 / 2(m_1 + m_2) \quad . \tag{IIIB4.4}$$

Equating the sum of Eqs. (IIIB4.3) and (IIIB4.4) to (IIIB4.1), and substituting (IIIB4.2), we find

$$E = \frac{k^2}{2m_1} + \frac{k^2}{2m_2} + \frac{2m_2 E}{2(m_1 + m_2)} \quad , \tag{IIIB4.5}$$

which reduces to

$$\frac{k^2}{2} = \left(\frac{1}{m_1} + \frac{1}{m_2} \right)^{-1} \frac{m_1}{m_1 + m_2} E \quad , \tag{IIIB4.6}$$

or

$$k^2 = 2m_2 \frac{m_1^2}{(m_1 + m_2)^2} E \quad . \tag{IIIB4.7}$$

This expression can be used to write Eq. (IIIB4.3), the energy in the com, in terms of the laboratory energy, as

$$E_{\text{in com}} = \frac{2m_2 m_1^2}{(m_1 + m_2)^2} \frac{E}{2m_2} + \frac{2m_2 m_1^2}{(m_1 + m_2)^2} \frac{E}{2m_1} = \frac{m_1 E}{(m_1 + m_2)} \tag{IIIB4.8}$$

The quantity k given in Eq. (IIIB4.7) corresponds to com incident momentum, required for the cross section formulae of Section III. The com momenta for other (non-incident) channels is also required, for use in the formulae for penetrabilities and shift factors. These momenta are found in similar fashion, using conservation of energy and momentum. Let k' represent the

momentum for a channel whose two masses are also denoted by primes. Then, in terms of primed quantities, the energy in the com is given by

$$E_{\text{in com}} = k'^2/2m'_1 + k^2/2m'_2 + Q_{\text{in com}} \quad , \qquad \text{(IIIB4.9)}$$

where Q is the threshold energy in the com system. Solving this equation for k' gives

$$k'^2 = \frac{2\,m'_1\,m'_2}{(m'_1+m'_2)}\,(E_{\text{in com}} - Q_{\text{in com}}) \quad . \qquad \text{(IIIB4.10)}$$

Combining this formula with Equation (IIIB4.8) gives k' in terms of the laboratory energy E,

$$k'^2 = \frac{2\,m'_1\,m'_2}{(m'_1+m'_2)}\,\frac{m_1}{(m_1+m_2)}\left(E - \frac{(m_1+m_2)}{m_1}\,Q_{\text{in com}}\right) \quad . \qquad \text{(IIIB4.11)}$$

Alternatively, if the laboratory Q-value is given, then

$$k'^2 = \frac{2\,m'_1\,m'_2}{(m'_1+m'_2)}\,\frac{m_1}{(m_1+m_2)}\left(E - Q_{\text{in lab}}\right) \quad . \qquad \text{(IIIB4.12)}$$

Note that in the SAMMY input, the user can specify the Q-value either in the laboratory system (as in Eq. (IIIB4.12)) or in the center-of-mass system (as in Eq. (IIIB4.11)); SAMMY will make the appropriate conversions. The default is laboratory. Users who wish to override the default (or who wish to keep a reminder handy) should include (in the INPut file) the phrase "LAB NON-COULOMB EXCITATION ENERGIES" or "CM NON-COULOMB EXCITATION ENERGIES" as needed for the non-Coulomb case, and "LAB COULOMB EXCITATION ENERGIES" or "CM COULOMB EXCITATION ENERGIES" for use with charged particle channels.

Within SAMMY, the conversion factors from laboratory energy to com momenta are calculated in subroutine fixrad in segment/subdirectory "old" (and also used in segment "new"), and stored in an array "zke" which must then be multiplied by the square root of the energy (minus the adjusted Q factor) to give k or k'. Appropriate numerical constants are included to facilitate conversion from units of eV (for energy) to inverse Fermi (for momentum). Values for constants are described in Appendix E of this report.

III.B.5 Derivative of One Complex Variable with Respect to Another

Given any two complex variables $A = A^r + iA^i$ and $B = B^r + iB^i$, where A is an analytical function of B, then the derivative of the components of A with respect to the components of B may be expressed as follows:

$$\frac{\partial A^r}{\partial B^r} = Re\,\frac{\partial A}{\partial B^r} = Re\,\frac{\partial A}{\partial B}\,\frac{\partial B}{\partial B^r} = Re\,\frac{\partial A}{\partial B} \quad ; \tag{IIIB5.1}$$

$$\frac{\partial A^r}{\partial B^i} = Re\,\frac{\partial A}{\partial B^i} = Re\,\frac{\partial A}{\partial B}\,\frac{\partial B}{\partial B^i} = Re\,\frac{\partial A}{\partial B}(i) = -\,Im\,\frac{\partial A}{\partial B} \quad ; \tag{IIIB5.2}$$

$$\frac{\partial A^i}{\partial B^r} = Im\,\frac{\partial A}{\partial B^r} = Im\,\frac{\partial A}{\partial B}\,\frac{\partial B}{\partial B^r} = Im\,\frac{\partial A}{\partial B} \quad ; \tag{IIIB5.3}$$

and

$$\frac{\partial A^i}{\partial B^i} = Im\,\frac{\partial A}{\partial B^i} = Im\,\frac{\partial A}{\partial B}\,\frac{\partial B}{\partial B^i} = Im\,\frac{\partial A}{\partial B}(i) = Re\,\frac{\partial A}{\partial B} \quad . \tag{IIIB5.4}$$

Also, the usual chain rule applies:

$$\frac{\partial A^r}{\partial C^r} = \frac{\partial A^r}{\partial B^r}\,\frac{\partial B^r}{\partial C^r} + \frac{\partial A^r}{\partial B^i}\,\frac{\partial B^i}{\partial C^r}$$

$$= \left[Re\,\frac{\partial A}{\partial B}\right]\left[Re\,\frac{\partial B}{\partial C}\right] + \left[-Im\,\frac{\partial A}{\partial B}\right]\left[Im\,\frac{\partial B}{\partial C}\right] = Re\left[\frac{\partial A}{\partial B}\,\frac{\partial B}{\partial C}\right] \quad ; \tag{IIIB5.5}$$

$$\frac{\partial A^r}{\partial C^i} = \frac{\partial A^r}{\partial B^r}\,\frac{\partial B^r}{\partial C^i} + \frac{\partial A^r}{\partial B^i}\,\frac{\partial B^i}{\partial C^i}$$

$$= \left[Re\,\frac{\partial A}{\partial B}\right]\left[-Im\,\frac{\partial B}{\partial C}\right] + \left[-Im\,\frac{\partial A}{\partial B}\right]\left[Re\,\frac{\partial B}{\partial C}\right] = -Im\left[\frac{\partial A}{\partial B}\,\frac{\partial B}{\partial C}\right] \quad ; \tag{IIIB5.6}$$

$$\frac{\partial A^i}{\partial C^r} = \frac{\partial A^i}{\partial B^r}\frac{\partial B^r}{\partial C^r} + \frac{\partial A^i}{\partial B^i}\frac{\partial B^i}{\partial C^r}$$

$$= \left[Im\frac{\partial A}{\partial B}\right]\left[Re\frac{\partial B}{\partial C}\right] + \left[Re\frac{\partial A}{\partial B}\right]\left[Im\frac{\partial B}{\partial C}\right] = Im\left[\frac{\partial A}{\partial B}\ \frac{\partial B}{\partial C}\right]; \qquad \text{(IIIB5.7)}$$

and

$$\frac{\partial A^i}{\partial C^i} = \frac{\partial A^i}{\partial B^r}\frac{\partial B^r}{\partial C^i} + \frac{\partial A^i}{\partial B^i}\frac{\partial B^i}{\partial C^i}$$

$$= \left[Im\frac{\partial A}{\partial B}\right]\left[-Im\frac{\partial B}{\partial C}\right] + \left[Re\frac{\partial A}{\partial B}\right]\left[Re\frac{\partial B}{\partial C}\right] = Re\left[\frac{\partial A}{\partial B}\ \frac{\partial B}{\partial C}\right]; \qquad \text{(IIIB5.8)}$$

III.D. ALTERNATIVE FORMULATION OF REICH-MOORE MULTILEVEL R-MATRIX THEORY

While the equations given in Section III.A.1 for the Reich-Moore approximation to multilevel R-matrix theory are correct, they may not be optimal for computer calculations. In particular, the calculation of the absorption or capture cross section at very low energies involves computation of a quantity having the form 1 - (1 - ε), where ε is small. This may result in large random fluctuations, the familiar "small difference of large numbers" problem. To circumvent this difficulty, the Reich-Moore equations have been programmed in an alternative manner: Starting from Eq. (IIIA1.12), the matrix W can be expressed in the form

$$W = I - 2i\ P\ L^{-1}\ (L^{-1}-R)^{-1}(L^{-1}-R) + 2i\ P^{1/2}\ L^{-1}\ (L^{-1}-R)^{-1}\ L^{-1}\ P^{1/2} \quad , \qquad \text{(III.D.1)}$$

which reduces to

$$W = I + 2i\ P^{1/2}\ L^{-1}(L^{-1}-R)^{-1}\ R\ P^{1/2} \quad , \qquad \text{(III.D.2)}$$

or, explicitly displaying the subscripts,

$$W_{cc'} = \delta_{cc'} + 2\,i\,P_l^{1/2}\,L_l^{-1} \sum_{c''} [(L^{-1}-R)^{-1}]_{cc''} R_{c''c'} P_{l'}^{1/2} \quad . \qquad \text{(III.D.3)}$$

If we define a matrix X such that

$$W = I + 2iX \quad , \qquad \text{(IIID.4)}$$

then X is given by

$$X_{cc'} = P_l^{1/2}\,L_l^{-1} \sum_{c''} [(L^{-1}-R)^{-1}]_{cc''} R_{c''c'} P_{l'}^{1/2} \quad . \qquad \text{(III.D.5)}$$

The absorption cross section can then be expressed in terms of X as

$$\sigma^{absorption}(E) = \frac{\pi}{k^2} \sum_J g_J \sum_c \left[1 - \sum_{c'} |\,(1+2iX)_{cc'}\,|^2\right] \quad , \qquad \text{(III.D.6)}$$

where c and c' are incident channels only. Letting X^r be the real part and X^i the imaginary part of X, this expresion becomes

$$\sigma^{absorption}(E) = \frac{\pi}{k^2} \sum_J g_J \sum_c \left[1 - \left(1 - 4X_{cc}^i + \sum_{c'} \{4X_{cc'}^{i\,2} + 4X_{cc'}^{r\,2}\}\right)\right] \quad , \qquad \text{(III.D.7)}$$

or

$$\sigma^{absorption}(E) = \frac{4\pi}{k^2} \sum_J g_J \sum_c \left[X_{cc}^i - \sum_{c'} \{X_{cc'}^{i\,2} + X_{cc'}^{r\,2}\}\right] \quad . \qquad \text{(III.D.8)}$$

Other cross sections (total, fission, elastic, etc.) can similarly be expressed in terms of matrix X. The fission (reaction) cross section becomes

$$\sigma^{reaction}(E) = \frac{4\pi}{k^2} \sum_J g_J \sum_{inc\ c} \sum_{exit\ c'} \{X^{i\ 2}_{cc'} + X^{r\ 2}_{cc'}\} \quad , \tag{III.D.9}$$

where the sums are over incident and exit channels, respectively. The capture cross section is

$$\sigma^{capture}(E) = \frac{4\pi}{k^2} \sum_J g_J \sum_{inc\ c} \left[X^i_{cc} - \sum_{all\ c'} \{X^{i\ 2}_{cc'} + X^{r\ 2}_{cc'}\} \right] . \tag{III.D.10}$$

The elastic cross section is given by

$$\begin{aligned} \sigma^{elastic}(E) = \frac{4\pi}{k^2} \sum_J g_J \sum_{inc\ c} \Big[& \sin^2\varphi_l\ (1 - 2X^i_{cc}) \\ & - X^r_{cc} \sin(2\varphi_l) + \sum_{inc\ c'} \{X^{i\ 2}_{cc'} + X^{r\ 2}_{cc'}\} \Big] . \end{aligned} \tag{III.D.11}$$

Finally the total cross section is the sum of all others, and can be written

$$\sigma^{total}(E) = \frac{4\pi}{k^2} \sum_J g_J \sum_{inc\ c} \left[\frac{1}{2} \sin^2\varphi_l + X^i_{cc} \cos(2\varphi_l) - X^r_{cc} \sin(2\varphi_l) \right] . \tag{III.D.12}$$

This formulation of the Reich-Moore equations has been implemented in segment XCT of the code SAMMY, and is now the default for all calculations. To override this default (i.e., to use the original formulation of the Reich-Moore equations), include the following card in the INPut file (See Table VIA.2):

ORIGINAL REICH-MOORE FORMULATION IS WANTED

Use of this (original) formulation is not permitted for certain types of data (e.g., differential elastic scattering, or capture yields with multiple-scattering corrections), and is discouraged in all cases.

Finally, note that the implementation of Eq. (III.D.9) has been generalized for Release M5 of the SAMMY code. Prior to M5, *all* exit channels were *always* included in the summation over *exit c'* channels, whenever "fission", "reaction", or "inelastic" cross sections were specified. With M5, however, it is now possible to exclude specified channels; details are given with the spin-group specifications for the INPut file (see parameter IFEXCL on Card 2 of Alternative to Card Set 10, page 108e). Thus one can now include, for example, inelastic and fission channels, and generate the inelastic cross section separately from the fission cross section. See test case tr93 for examples of this feature.

III.F SELF-SHIELDING AND MULTIPLE-SCATTERING CORRECTIONS TO CAPTURE OR FISSION YIELDS

The theoretical capture or fission cross section may be calculated directly from Eq. (IIIA1.5) using the Reich-Moore (or other) approximation to the multilevel R-matrix. However, in order to compare with experiment, corrections must be made for the finite (non-infinitesimal) size of the sample. Both "self-shielding" and "multiple-scattering" effects must be included in the calculation. [Note: to avoid arduous repetition, for the rest of this section "capture" will be taken to mean "capture or fission"; the corrections described here apply to both.]

Derivation of the appropriate expressions for self-shielding and multiple-scattering corrections, and details of the methods of calculation, will be presented in a separate publication [NL01]. Included in that publication will be a description of validity tests of formulae in this section, and of their implementation within SAMMY, using Monte-Carlo techniques. Preliminary results of those tests indicate good agreement between Monte-Carlo results and results obtained via SAMMY.

Self-Shielding

Self-shielding is the reduction in the observed capture cross section due to interactions of incident neutrons with other nuclei in front of the current position. The probability that capture will occur at depth z (within dz) can be written as

$$\frac{n}{D}\, e^{-n\sigma_t z/D}\, \sigma_c\, dz \quad , \tag{IIIF.1}$$

where n is the sample thickness in atoms/barn and D is the sample thickness in the same units as z. Subscripts t and c denote total and capture cross sections, respectively. Integrating over z (from 0 to D) gives the self-shielded capture yield

$$Y_0 = \left\{ 1 - e^{-n\sigma_t} \right\} \left(\frac{\sigma_c}{\sigma_t} \right) \quad . \tag{IIIF.2}$$

(See the end of this section for a discussion of the normalization options for capture yields.)

Single-Scattering

The scattering correction is the increase in the observed capture cross section due to capture of neutrons that have been scattered out of the original beam path. Calculation of the scattering effect is more complicated than the self-shielding, because it involves the product of (1) the probability of reaching a position (x,y,z) inside the sample, (2) the probability of scattering from

that position into solid angle Ω within $d\Omega$, (3) the probability of those scattered nuclei reaching position q within dq along that direction, and (4) the probability of being captured at that location. This product is then integrated over the position q, over solid angle, and over the sample volume, giving the *single*-scattering result. If the z-axis is defined by the beam line, this expression can be reduced to the form

$$Y_1(E) = \frac{\int dx \int dy}{S} \frac{n}{D} \int dz \exp(-\frac{n}{D}\sigma_t z) \int d\Omega \frac{d\sigma}{d\Omega} \sigma_c' \frac{n}{D} \int dq \exp(-\frac{n}{D}\sigma_t' q) \ , \quad \text{(IIIF.3)}$$

in which primes indicate evaluation at the scattered energy, rather than at the incident energy of the neutron. The scattered energy is given by

$$E' = E\left[\frac{\cos\theta}{(1+r)} + \sqrt{\frac{1}{(1+1/r)^2} - \frac{\sin^2\theta}{(1+r)^2}}\right]^2 = E\,\varepsilon(\theta) \ , \quad \text{(IIIF.4)}$$

where r is the ratio of the mass of the target nuclide to the mass of the neutron.

Explicit evaluation of the expression in Eq. (IIIF.3) requires detailed knowledge of the geometry of the sample and its positioning relative to the neutron beam. In the case where the sample is a round disk, with a flat surface perpendicular to the beam, the expression can be reduced to

$$Y_1(E) = Y_{1\infty f} + Y_{1\infty b} + Y_{1\not\infty f} + Y_{1\not\infty b} \ , \quad \text{(IIIF.5)}$$

where the subscripts "f" and "b" refer to forward and backward scattering, respectively. The subscript ∞ indicates that this term assumes the sample extends to infinity in the dimensions perpendicular to the beam; subscript $\not\infty$ indicates that this term is the correction for finite size. (NOTE: Corrections for a rectangular shape, rather than a round disk, will be available in future releases of the code.)

The "infinite" terms in Eq. (IIIF.4) are one-dimensional integrals,

$$Y_{1\infty f}(E) = \frac{1}{2}\int_0^1 d\mu \frac{d\sigma}{d\Omega} \frac{\sigma'_{cap}}{\sigma'_{tot}} \left(\frac{1-e^{-n\sigma_{tot}}}{\sigma_{tot}} + \frac{e^{-n\sigma_{tot}} - e^{-n\sigma'_{tot}/\mu}}{\sigma_{tot} - \sigma'_{tot}/\mu} \right) , \quad \text{(IIIF.6)}$$

$$\text{and} \quad Y_{1\infty b}(E) = \frac{1}{2}\int_{-1}^0 d\mu \frac{d\sigma}{d\Omega} \frac{\sigma'_{cap}}{\sigma'_{tot}} \left(\frac{1-e^{-n\sigma_{tot}}}{\sigma_{tot}} - \frac{1-e^{-n(\sigma_{tot}-\sigma'_{tot}/\mu)}}{\sigma_{tot} - \sigma'_{tot}/\mu} \right) , \quad \text{(IIIF.7)}$$

in which $\mu=\cos(\theta)$. The "finite" corrections involve four-dimensional integrals of the form

$$Y_{1*f}(E) = \int_0^1 d\mu \, \frac{d\sigma}{d\Omega} \, \frac{\sigma'_{cap}}{\sigma'_{tot}} \, Q_f(\mu, \sigma_{tot}, \sigma'_{tot}) \qquad \text{(IIIF.8)}$$

$$\text{and } Y_{1*b}(E) = \int_{-1}^0 d\mu \, \frac{d\sigma}{d\Omega} \, \frac{\sigma'_{cap}}{\sigma'_{tot}} \, Q_b(\mu, \sigma_{tot}, \sigma'_{tot}) \ , \qquad \text{(IIIF.9)}$$

in which the three-dimensional integral Q_f is given by

$$Q_f(\mu, \sigma, \sigma') = \int dz \, e^{-n\sigma' \frac{D}{z}} \int d^2S \left(e^{-n\sigma(D-z)/(D\mu)} - e^{-n\sigma L/D} \right) , \qquad \text{(IIIF.10)}$$

and Q_b by

$$Q_b(\mu, \sigma, \sigma') = \int dz \, e^{-n\sigma' \frac{D-z}{z}} \int d^2S \left(e^{-n\sigma(D-z)/(D\mu)} - e^{-n\sigma L/D} \right) , \qquad \text{(IIIF.11)}$$

where L is the actual path length, within the sample, available for travel by the scattered neutron; note that L is geometry-dependent. The integration over d^2S in this expression for Q is over the beam cross section; the integration over z is over the thickness of the sample. SAMMY evaluates Q on a separate grid and interpolates to produce the required values for Eqs. (IIIF.7-8).

Values for Q are generated in advance (in segment SAMPAR) and stored in a file named SAMMY.SSM. This file may be renamed and reused for subsequent runs, so long as the geometry remains the same.

Two or More Scatters

Derivation of the effect of two or more scatters followed by capture is accomplished in a similar manner to the derivation of the single-scattering effect. The exact expression for k scatters involves $(3k+3)$ embedded integrations; it is therefore necessary to make severe approximations in order to derive an expression which can be calculated in a finite amount of time. The approximation currently employed by SAMMY is borrowed from Moxon [MM89], based on a derivation by Case et al. [KC53]; an independent derivation is presented in [NL99a]. The approximation assumes that after two scatterings, neutrons are uniformly distributed both in direction of motion and in position within the sample. This approximation has the effect of decoupling $2k$ of the embedded integrals, so that they can be performed separately from the others. Quantization of this approximation is achieved by assuming that the escape probability for a neutron after k scatterings (i.e., at energy $E^{(k)}$) depends only on the energy; specifically, the escape probability is given by the formula

$$p_{escape}(E^{(k)}) = \frac{1}{n\sigma^{(k)}}\left[\frac{1}{2} - \int_1^\infty u^{-3}\,du\; e^{-n\sigma^{(k)}u}\right] \times \frac{1+2n\sigma_t^{(k)}}{1+\dfrac{2n\sigma_t^{(k)}}{1+Z/R}} \quad , \qquad \text{(IIIF.12)}$$

where R is the radius of the sample. With this approximation, one can recursively define a function y via

$$y_{j-1} = \int d\Omega_j \frac{d\sigma^{(j-1)}}{d\Omega_j}\left(\sigma_c^{(j)} + y_j\right)\left(1 - p_{escape}(E^{(j)})\right) \quad , \qquad \text{(IIIF.13)}$$

in which the superscript denotes the energy at which the cross section is to be calculated. The initial estimate for a neutron scattered k times is

$$y_{k-1} \approx 2\pi \int d\mu_k \frac{d\sigma^{(k-1)}}{d\Omega_k}\,\sigma_c^{(k)}\left(1 - p_{escape}(E^{(k)})\right) \quad . \qquad \text{(IIIF.14)}$$

This function y can then be used to estimate the capture yield for two or more scatterings,

$$\bar{Y}_2(E) = \frac{\int dx \int dy}{S}\,\frac{n}{D}\int dz\; e^{-\frac{n}{D}\sigma_t z}\int d\Omega\,\frac{d\sigma}{d\Omega}\,y_1\,\frac{n}{D}\int dq\; e^{-\frac{n}{D}\sigma_t' q} \quad . \qquad \text{(IIIF.15)}$$

In this form the multiple-scattering capture yield has the same mathematical properties as the single-scattering capture yield of Eq. (IIIF.3). Similar computational techniques can therefore be used to evaluate both quantities.

Normalization and Input Options

Capture yield data may be normalized in a variety of ways; therefore SAMMY allows the user to choose which normalization is to be taken. The normalization generally referred to as capture "yield" is the one shown in the equations in this section; this choice has the property that values are in the range from 0 to 1. Another commonly used normalization requires dividing by thickness n; in this case the value approaches the capture cross section in the limit of zero thickness. Finally, the data may be normalized as $(1 - e^{-n\sigma_t})\,\sigma_t$, that is, by multiplying the yield by the total cross section. To use these options, the user must include the appropriate phrase in the alphanumeric section of the INPut file:

```
NORMALIZE AS CROSS Section rather than yield
NORMALIZE AS YIELD Rather than cross section
NORMALIZE AS (1-E)SIgma
```

No default is assumed for normalization; instead, SAMMY requires that one of the above options be specified by the user.

The default mode in SAMMY is to not include self-shielding and multiple-scattering corrections; therefore, to invoke these corrections, users will need to include one or more of the following phrases in their INPut file:

For self-shielding but no multiple-scattering:

```
USE SELF SHIELDING Only, no scattering, or
SELF SHIELD
```

For self-shielding, single-scattering (with edge-effects correction), and no double-scattering:

```
USE SINGLE SCATTERINg plus self shielding, or
SINGLE
```

For self-shielding, single-scattering (infinite slab approximation), and no double-scattering:

```
SINGLE
INFINITE SLAB
```

For self-shielding, single-scattering (with edge-effects correction), and multiple-scattering:

```
USE DOUBLE SCATTERINg plus single scattering, or
DOUBLE
```

For self-shielding, single-scattering (infinite-slab approximation), and multiple-scattering:

```
DOUBLE
INFINITE SLAB
```

When finite-size corrections (for single-scattering) are wanted, additional input is needed to express the geometric properties of the beam and of the sample. These include the dimensions of the sample, the cross-sectional dimensions of the beam if different from and smaller than the sample, and integers that determine the accuracy to which the function Q will be calculated. Details are given in Table VIA.1, Card Set 11.

Examples using multiple-scattering corrections can be found in test cases tr39, tr52, tr64, and tr99.

III.H. COULOMB PENETRABILITIES

The penetrabilities P_l, shift factors S_l, and potential scattering phase shifts φ_l defined in Table IIIA1.1 apply only to non-Coulomb interactions such as those involving incident neutrons. Often, however, the two particles in a channel will both have a positive charge; examples are the exit channels for (n,α) or (n,p) interactions, and the incident channels in the reciprocal measurements (α,n) and (p,n). In this case the expressions for penetrabilities, shift factors, and phase shifts must be modified to include the long-range interaction; see, for example, the discussion of Lane and Thomas [AL58].

An extension for SAMMY to include Coulomb interactions has been developed by R. Sayer [RS00] (and modified slightly by the SAMMY author), and used first for analysis of ^{16}O data [LL98, RS00]. FORTRAN routines used for this purpose are a modified version of the routine COULFG of Barnett [AB82].

Expressions for P_l, S_l, and φ_l for channel c involve a parameter η_c, which is defined as

$$\eta_c = \frac{Z_1 Z_2 e^2 \mu_{1,2}}{\hbar^2 k_c} \qquad \text{(IIIH.1)}$$

where Z_i is the charge number for particle number i in channel c. The reduced mass $\mu_{1,2}$ is defined in the usual manner as

$$\mu_{1,2} = \frac{m_1 m_2}{m_1 + m_2} \qquad \text{(IIIH.2)}$$

where m_i is the mass of the ith particle in channel c. The center-of-mass momentum k_c is defined in the same manner as in Eq. (IIIB4.12),

$$k_c^2 = \frac{2 m_1 m_2}{(m_1 + m_2)} \frac{m_1^{inc}}{(m_1^{inc} + m_2^{inc})} (E_{lab} - Q_{lab}) \quad . \qquad \text{(IIIH.3)}$$

in which the masses of particles in the incident channel are denoted by a superscript, since they may be different from the masses in channel c. Alternatively, if the Q-value is given in the center-of-mass system, this expression takes the form as given in Eq. (IIIB4.11),

$$k_c^2 = \frac{2 m_1 m_2}{(m_1 + m_2)} \frac{m_1^{inc}}{(m_1^{inc} + m_2^{inc})} \left(E_{lab} - \left[\frac{(m_1^{inc} + m_2^{inc})}{m_1^{inc}} \right] Q_{in\ com} \right) \quad . \qquad \text{(IIIH.4)}$$

Note that in the SAMMY input, the user can specify the Q-value either in the laboratory system (as in Eq. (IIIH.3)) or in the center-of-mass system; SAMMY will make the appropriate conversions. The default is laboratory. Users who wish to provide com values should include the phrase "CM COULOMB EXCITATION ENERGIES" as needed. (The reaction Q-value is input as variable ECHAN in Card Set 9 or Alternative to Card Set 10 as described on pages 108a and 108f.)

The penetrabilities $P_l(\eta,\rho)$, shift factors $S_l(\eta,\rho)$, and phase shifts $\varphi_l(\eta,\rho)$ are then calculated as functions of $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$, the regular and irregular Coulomb wave functions respectively. The equations are as follows:

$$P_l = \frac{\rho}{A_l^2}, \qquad S_l = \frac{\rho}{A_l}\frac{\partial A_l}{\partial \rho}, \qquad \text{and} \qquad \cos\varphi_l = \frac{G_l}{A_l}, \tag{IIIH.5}$$

where

$$A_l^2 = F_l^2 + G_l^2 \qquad \text{and} \qquad \rho = k_c\, a_c \ : \tag{IIIH.6}$$

the quantity a_c is the channel radius.

IV.A.2.c. Resolution broadening: Convolution of Gaussian and Exponential

Gaussian and exponential resolution broadening may be invoked simultaneously, giving the broadened cross section (or transmission) as

$$f_{GE}(E) = \frac{1}{\Delta_E \Delta_G \sqrt{\pi}} \int_{E-\Delta E_S}^{\infty} dE^o \exp\left\{-\frac{\left(E^o-(E-\Delta E_S)\right)}{\Delta_E}\right\} \times \int_{t}^{\infty} dE' \exp\left\{-\frac{(E'-E^o)^2}{\Delta_G^2}\right\} f(E') \quad , \tag{IVA2c.1}$$

where the shift ΔE_S is introduced in order that the maximum of the broadening function be located at $E' = E$.

Rearrangement of the integrands in Eq. (IVA2c.1) and explicit integration over the E^o variable yield

$$f_{GE}(E) = \frac{1}{2\Delta_E} \int_{E}^{\infty} dE' f(E') \exp\left\{-\frac{(E'-E+\Delta E_S)}{\Delta_E}\right\} \times \mathrm{erfc}\left(\frac{\Delta_G}{2\Delta_E} - \frac{(E'-E+\Delta E_S)}{\Delta_E}\right) \quad . \tag{IVA2c.2}$$

Historical Note: this is not the form which is given in the MULTI manual [GA74], but is the (correct) form that is used in both the MULTI and the SAMMY code.

The energy shift ΔE_S is found by setting $g(E') = \exp(.)\,erfc(.)$ from the integrand of Eq. (IVA2c.2), and locating the value of E_{max}' for which $g(E_{max}')$ is a maximum by setting $dg/dE' = 0$ at that value. This value E_{max}' is then set equal to E, and the resulting equation solved for ΔE_S. Newton's method is used to find the solution.

Alternatively, one can assume that the energy shift is zero. This requires the inclusion of a card in the INPut file reading

```
DO NOT SHIFT ENERGY for exponential tail on resolution broadening
```

The lower and upper integration limits in Eq. (IVA2c.2) are truncated to $E - 5\Delta_G$ and max $(E + 6.25\,\Delta_E,\ E + 5\Delta_G)$, respectively.

IV.B. EVALUATING BROADENING INTEGRALS

SAMMY's method of evaluating the integrals required in Doppler and resolution broadening involves several operations for which details are given in the subsequent subsections. The method was borrowed originally from the MULTI code [GA74] and subsequently modified as the need arose. Note that in SAMMY, broadening is applied both to the cross sections and to the derivatives, while in MULTI it was applied only to the cross sections. A summary of the operations is given here:

1. Choose an appropriate "auxiliary energy grid" at which to evaluate the integrands. The auxiliary grid consists of (a) the original energy grid (i.e., the energies at which experimental data are given), (b) points below the minimum energy of the experimental data and above the maximum energy, and (c) additional points sufficient to describe the structure of any "narrow" resonance. See Sect. IV.B.1 for more details. [Different criteria are required for Leal-Hwang Doppler broadening; see Sect. IV.A.3.]

2. Evaluate the theoretical cross section and derivatives thereof for each energy in the auxiliary grid.

3. Determine Doppler-broadened cross section and derivatives wherever possible (that is, for all but the highest and the lowest energies in the auxiliary grid). Generate derivatives with respect to Doppler temperature.

4. Transform from cross section to transmission as needed; apply transformation to derivatives also. See Sect. V.A. Generate derivative with respect to thickness.

5. Apply self-shielding and multiple-scattering corrections as needed, both to cross sections and to derivatives. See Sect. III.F.

6. For each energy in the original (experimental) grid, determine the resolution-broadened cross section (or transmission) and derivatives thereof. Also generate derivatives with respect to resolution-broadening parameters.

7. If needed, transform from transmission back to cross section; transform derivatives also.

8. Multiply by normalization and add backgrounds, as needed. Generate derivatives with respect to normalization and background.

IV.G RPI RESOLUTION BROADENING

Researchers at Rensselaer Polytechnic Institute (RPI) have carefully measured the resolution function associated with the "bounce target" and the transmission detector (Li glass) for the LINAC at RPI [BM96]. This resolution function may be described by the sum of a chi-squared function (with six degrees of freedom) plus two exponential terms. The total resolution function appropriate for data measured on that machine is then the convolution of the target-detector resolution function with a Gaussian function representing the electron burst and a square function representing the channel width.

Within SAMMY, this resolution function is formed in much the same manner as described for the realistic resolution function of Section IV.E, i.e., the resolution-broadened cross section $\bar{\sigma}(t)$ may be expressed as

$$\bar{\sigma}(t) = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2 \int I_3(t_2-t_3)\,dt_3\ \sigma(t_3) \quad , \tag{IVG.1}$$

where I_i is our mathematical model for the ith component. This expression may then be rearranged into the form

$$\bar{\sigma}(t) = \int I(t-t')\ \sigma(t')\,dt' \quad , \tag{IVG.2}$$

where the resolution function $I(t-t')$ is defined as

$$I(t-t') = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2\ I_3(t_2-t') \quad . \tag{IVG.3}$$

Because SAMMY deals with cross sections as functions of energy, rather than time, the relationship

$$E = \frac{1}{2}mv^2 = \frac{1}{2}m\frac{L^2}{t^2} \tag{IVG.4}$$

is used to convert from energy to time and *v.v.* in Eq. (IVG.2), yielding

$$\bar{\sigma}(E) = \int I'(t(E)-t')\ \sigma(E'(t'))\,dt' \quad . \tag{IVG.5}$$

In the following section the component functions I_i are described, along with the parameters for those components. Complete details will be presented in a separate report [NL99c].

Test Case Tr53, Tr54, Tr94, and Tr95 show several examples using the RPI resolution function, with parameter values suitable both for RPI data and for Geel data. To make plots of this resolution function and the individual components, see Section VIII.M, page 150z.3.

IV.G.1 Description of the Components of the RPI Resolution Function

1. Electron Burst

The electron burst from the RPI linac may be described by a Gaussian function in time, of the form:

$$I_1(t) = \frac{w}{\sqrt{\pi}}\, e^{-w^2 t^2} \quad , \tag{IVG1.1}$$

where $2\sqrt{\ln 2}\,/w = p$ is the full width at half max of the burst. Normalization is unity for this function.

2. Target plus Detector

The RPI transmission resolution function, which represents the combined components for the "bounce target" and transmission detector, has been found by RPI researchers [BM96] to be best described by the sum of a chi-squared function with six degrees of freedom plus two exponential terms. A similar function (with different values for the parameters) describes the bounce target plus capture detector. Specifically, this function has the form

$$I_2(t) = A_0 \left\{ \frac{(t+\tau)^2}{2!\,\Lambda^3}\, e^{-(t+\tau)/\Lambda} + A_1 \left[A_2\, e^{-A_3 (t+t_0)} + A_4\, e^{-A_5 (t+t_0)} \right] X(t) \right\} , \tag{IVG1.2}$$

in which the function $X(t)$ is zero if the quantity within the square brackets (the sum of the exponential terms) is negative, and unity otherwise. Likewise the χ^2 function is assumed to have zero value when the exponent is positive (i.e., when $t + \tau < 0$). The value of A_0 is chosen to give an overall normalization of unity for this function. Parameters Λ, τ, and A_1 are functions of energy, the specific forms being

$$\Lambda(E) = \Lambda_0 + \Lambda_1 \ln(E) + \Lambda_2 [\ln(E)]^2 + \Lambda_3\, E^{\Lambda_4} \tag{IVG1.3}$$

for Λ,

$$\tau(E) = \tau_1\, e^{-\tau_2 E} + \tau_3\, e^{-\tau_4 E} + \tau_5 + \tau_6\, E^{\tau_7} \tag{IVG1.4}$$

for τ, and

$$A_1(E) = a_1\, e^{-a_2 E} + a_3\, e^{-a_4 E} + a_5 + a_6\, E^{a_7} \tag{IVG1.5}$$

for A_1. All other quantities in Eq. (IVG1.2) are independent of energy.

Input formats for all parameters are given in Table VIB.1 Card Set 14 starting on page 122s; note that zero values are assumed to actually be zero and are not replaced by default values. In Table IVG1.1, default values for the constants from Eq. (IVG1.2) through (IVG1.5) are defined for transmission and capture measurements; to invoke these defaults, the user must specify "RPI Transmission resolution function" or "RPI Capture resolution function" on the first line of Card Set 14. See Test Case TR53 and TR54 for sample input for the RPI resolution function.

Table IVG1.2, provided courtesy of Frank Gunsing of Saclay [FG00], gives values of parameters that may be suitable for use with data from GELINA. See also Test Case TR94 and (especially) TR95 for sample input. Note that these values are *preliminary*; they are reasonable starting values which should be fine-tuned on measurements of well-known resonances (i.e. measured many times at different installations). The reader should also be aware that an extension of the formulae (to include a third exponential term) is planned for the near future; the extension is expected to improve the description of the resolution function above 1 keV.

3. Time-of-Flight Channel Width

The time-of-flight channel width may be modeled as a rectangular distribution of width c. The time distribution due to the finite channel width is therefore assumed to be:

$$I_3(t) = \begin{cases} 1/c & for \ -c/2 < t < c/2 \\ 0 & otherwise \end{cases}, \qquad \text{(IVG1.6)}$$

where the channel width c may be different for different energy-regions.

Table IVG1.1. Default values for parameters for RPI resolution function.

	Parameter name	Value for transmission "RPI Transmission"	Value for capture[a] "RPI Capture"	Units
1	$p = 2\sqrt{\ln 2}/w$			ns
2	τ_1	326.	381.	ns
3	τ_2	0.0241	0.0058	per eV
4	τ_3	323.	323.	ns
5	τ_4	0.029	0.094	per eV
6	τ_5	240.	105.	ns
7	τ_6	0.	0.	ns
8	τ_7	0.	0.	[dimensionless]
9	Λ_0	686.5	686.5	ns
10	Λ_1	-224.9	-224.9	ns
11	Λ_2	21.04	21.04	ns
12	Λ_3	0.	0.	ns
13	Λ_4	0.	0.	[dimensionless]
14	a_1	-0.000985	-0.001106	per ns
15	a_2	0.0241	0.0058	per eV
16	a_3	-0.000626	0.04752	per ns
17	a_4	3.531	65.083	per eV
18	a_5	0.001029	0.001264	per ns
19	a_6	0.	0.	per ns
20	a_7	0.	0.	[dimensionless]
21	t_0	940.	940.	ns
22	A_2	-65.638	-65.638	[dimensionless]
23	A_3	0.005	0.005	per ns
24	A_4	0.39383	0.39383	[dimensionless]
25	A_5	0.0008	0.0008	per ns
26	c			ns

[a] Values listed in this column are *not* necessarily those which are appropriate for the RPI capture resolution function, which has not yet been fully defined; these values are for illustrative purposes only.

Table IVG1.2. Parameters suitable for use with experimental data from the Geel Linac. Values are from preliminary work of F. Gunsing [FG00].

	Parameter name	Value for transmission	Value for capture	Units
1	$p = 2\sqrt{\ln 2}/w$			ns
2	τ_1	0.0	0.0	ns
3	τ_2	0.0	0.0	per eV
4	τ_3	0.0	0.0	ns
5	τ_4	0.0	0.0	per eV
6	τ_5	0.0	0.0	ns
7	τ_6	-353.0185	-11.406	ns
8	τ_7	-0.4307	0.1699	[dimensionless]
9	Λ_0	1.6809	1.7606	ns
10	Λ_1	0.0	0.0	ns
11	Λ_2	0.0	0.0	ns
12	Λ_3	472.8168	450.8649	ns
13	Λ_4	-0.4952	-0.4992	[dimensionless]
14	a_1	-0.1062	-0.8104	per ns
15	a_2	0.0040555	0.00014562	per eV
16	a_3	0.0	0.0	per ns
17	a_4	0.0	0.0	per eV
18	a_5	0.1061	0.8102	per ns
19	a_6	0.00020477	0.0006135	per ns
20	a_7	0.7517	0.5348	[dimensionless]
21	t_0	-1.5	-1.5	ns
22	A_2	0.0030464	0.0030464	[dimensionless]
23	A_3	0.002351	0.02351	per ns
24	A_4	0.00022682	0.0002682	[dimensionless]
25	A_5	0.0069803	0.0069803	per ns
26	c			ns

V. SPECIAL TREATMENTS

This section is our "junk drawer," containing information on a variety of topics which did not seem to fit well into any particular category. Included here are discussions of SAMMY's treatment of transmission data (Section V.A), and of the handling of correlated data sets (Section V.B). Section V.C describes how SAMMY may be used to average cross sections (both theoretical and experimental) over an energy range after the analysis is complete, in order to compare with other experimental data. The means by which one may analyze samples containing multiple nuclides (mutiple isotopes, chemical compounds, contaminants) are discussed in Section V.D. Section V.E is devoted to two methods of including data-reduction parameters within the SAMMY analysis. Maxwellian averages of capture cross sections (sometimes called "stellar averages") are discussed in Section V.F. Methods for reconstructing point-wise cross sections without having to specify an energy grid are given in Section V.G. Paramagnetic cross sections are discussed in Section V.H. Section V.I includes a disccussion of integral quantities. Fröhner's treatment of the unresolved region, now introduced as a part of the SAMMY code, is described in Section V.J. A treatment of l-dependent detector efficiencies is outlined in Section V.K. The treatment of individual reactions types as final states (e.g., inelastic separate from (α,n) reactions) is described in Section V.L.

V. C AVERAGING THE CROSS SECTIONS

Once the SAMMY analysis is completed, the analyst may wish to average the theoretical curves produced by SAMMY over an energy range (or ranges) in order to more directly compare his/her results with those from other experiments or analyses. Or s/he may wish to produce multi-group cross sections plus covariance matrix for use in further calculations.

Two options are available in SAMMY for averaging the cross section. The original option uses a energy- or time-average; see Sect. V.C.1. The second uses the Bondarenko [IB64] narrow-resonance scheme; see Sect. V.C.2. In both cases, uncertainties are propagated through the entire procedure, resulting in correct uncertainties and correlation matrix for the multi-group cross sections.

V. C.1 Energy- or Time-Weighted Averages

The averaged cross section is defined as

$$\bar{\sigma} = \frac{1}{N} \int_{Emin}^{Emax} \sigma(E')\, W(E')\, dE' \quad , \tag{VC1.1}$$

in which the weight factor $W(E')$ specifies how the averaging is to be performed and in which the normalization N is given by

$$N = \int_{Emin}^{Emax} W(E')\, dE' \quad . \tag{VC1.2}$$

In practice the integrals in Eqs. (VC1.1) and (VC1.2) are replaced by sums over discrete intervals of the form

$$\bar{\sigma} = \frac{1}{N} \sum_{i=Imin}^{Imax} \sigma_i \Delta_i \quad , \tag{VC1.3}$$

with N given by the same formula with the σ_i term omitted inside the summation. The Δ_i may have any of several possible values, corresponding to different interpretations of the averaging process. Two possibilities are available in SAMMY: energy-averaging and time-averaging. In the first of these, the Δ_i are given by

$$\Delta_i = \frac{1}{2}\left[E_{i+1} - E_{i-1}\right] \quad , \tag{VC1.4}$$

which is equivalent to assuming the channel end-points are exactly half-way between the energies specified as channel energy.

The second option for averaging the theoretical curve in SAMMY is to time-average, in which case the Δ_i are given by the difference between the time at the end of a channel and the time at the beginning. This assumes that the specified experimental energies are stated at the center of the channel, i.e., that the time associated with channel i is

$$t_i = \sqrt{\frac{m}{2}\frac{L^2}{E_i}} \tag{VC1.5}$$

and the Δ_i are then given by

$$\Delta_i = \frac{1}{2}\left[t_{i+1} - t_{i-1}\right] \quad . \tag{VC1.6}$$

In both cases described above, corrections are made to ensure that the range included in the summation does not extend beyond the minimum and maximum energies, which are not likely to be channel boundaries. Note that neither of these approximations is exactly correct when compared to the experimental situation, since the end-points of the time-of-flight channels are estimated based on center-time information. A more correct procedure would be to use the exact information from the experimental time-of-flight channels; unfortunately such information is not available to the analysis.

To determine the uncertainties associated with $\bar{\sigma}$, we consider a small increment in $\bar{\sigma}$, which can be written as

$$\delta\bar{\sigma} = \frac{1}{N}\sum_j \sum_i \frac{\partial \sigma_i}{\partial u_j}\,\Delta_i\,\delta u_j \quad , \tag{VC1.7}$$

where u_j are the u-parameters (see Sect. II.C). Squaring this quantity and taking expectation values gives the variance on $\bar{\sigma}$ as

$$\begin{aligned} var(\bar{\sigma}) &= <(\delta\bar{\sigma})^2> \\ &= \frac{1}{N^2}\sum_i\sum_{i'}\sum_j\sum_{j'}\frac{\partial \sigma_i}{\partial u_j}\frac{\partial \sigma_{i'}}{\partial u_{j'}}\,\Delta_i\,\Delta_{i'}\,<\delta u_j \delta u_{j'}> \quad . \end{aligned} \tag{VC1.8}$$

Note that the quantity $<\delta u_j \delta u_{j'}>$ is just the parameter covariance matrix $M_{jj'}$, which is known from the earlier analysis. The partial derivatives in Eq. (VC1.8) are readily evaluated within SAMMY, and the Δ_i are known. Thus, the uncertainty on the average cross section $\bar{\sigma}$ may be found directly from this equation.

The input needed to use this option is described in Sect. VI.E. Examples are given in test cases tr14 and tr75.

V.C.2 Bondarenko-Weighted Averages

The general definition of the flux-weighted multigroup cross section is

$$\bar{\sigma}_{x,i} = \int_{E_i^g}^{E_{i+1}^g} \sigma_x(E)\ \Phi(E)\ dE \Bigg/ \int_{E_i^g}^{E_{i+1}^g} \Phi(E)\ dE \qquad \text{(VC2.1)}$$

in which subscript x indicates the particular type of cross section (e.g. capture, fission, total). [Superscript g on the energy limits is used to distinguish these energies from the energies E_i of the experimental grid.] The flux $\Phi(E)$ is the energy-dependent neutron flux. Since this flux is not known, the Bondarenko narrow-resonance scheme [IB64] is often used. This scheme is defined as

$$\bar{\sigma}_{x,i} = \int_{E_i^g}^{E_{i+1}^g} \frac{\sigma_x(E)\ C(E)}{\sigma_t(E) + \sigma_0}\ dE \Bigg/ \int_{E_i^g}^{E_{i+1}^g} \frac{C(E)}{\sigma_t(E) + \sigma_0}\ dE \qquad \text{(VC2.2)}$$

in which σ_t is the total cross section, σ_0 is an energy-independent constant, and $C(E)$ is a smooth function of energy. Currently in SAMMY, $C(E)$ may be expressed as a piece-wise linear function of energy; see Section VI.E for input options.

The limit in which C is constant and σ_0 is effectively infinite,

$$\bar{\sigma}_{x,i} = \int_{E_i^g}^{E_{i+1}^g} \sigma_x(E)\ dE \Bigg/ \int_{E_i^g}^{E_{i+1}^g} dE\ , \qquad \text{(VC2.3)}$$

is the form implemented elsewhere (see Section V.C.1) as "energy averages" in SAMMY.

In addition to the calculating the multigroup cross sections, it is also necessary to generate the associated covariance matrix. This is accomplished by first taking small increments

$$\delta\bar{\sigma}_{x,i} = \sum_k \frac{\partial\bar{\sigma}_{x,i}}{\partial u_k}\ \delta u_k\ , \qquad \text{(VC2.4)}$$

where u represents the resonance parameters. The covariance matrix is then found by taking expectation values

$$C_{i,j} = < \delta \bar{\sigma}_{x,i} \, \delta \bar{\sigma}_{x,j} > = \sum_{k,k'} \frac{\partial \bar{\sigma}_{x,i}}{\partial u_k} < \delta u_k \, \delta u_{k'} > \frac{\partial \bar{\sigma}_{x,j}}{\partial u_{k'}} = \sum_{k,k'} \frac{\partial \bar{\sigma}_{x,i}}{\partial u_k} M_{k,k'} \frac{\partial \bar{\sigma}_{x,j}}{\partial u_{k'}} \quad , \quad \text{(VC2.5)}$$

in which

$$M_{k,k'} = < \delta u_k \, \delta u_{k'} > \quad \text{(VC2.6)}$$

is the (known) covariance matrix for the resonance parameters.

Derivatives of the multigroup cross sections with respect to the resonance parameters are found using the chain rule, in the usual fashion. Details will be presented elsewhere [NL01a], as will details of the implementation of these equations within SAMMY.

Input needed to generate Bondarenko-weighted averages (multigroup cross sections) and covariance matrix using SAMMY is described in Section VI.E of this document. Examples are given in Test Cases tr83 and tr85; included in these examples are validity tests where the Bondarenko scheme of Eq. (VC2.2) is used to mimic the energy-average scheme of Section V.C.1 and Eq. (VC2.3).

V. E. 1 Explicit Normalization and/or Background Functions

A constant overall normalization and a variety of different analytical models for backgrounds may be applied to the theoretical values (cross sections, transmissions, etc.) generated within SAMMY. These corrections are applied to the theory, not to the data. Normalization is applied first, followed by background corrections, so that the backgrounds are not multiplied by the normalization.

Let T_u represent the uncorrected theoretical value (for cross section, transmission, etc.); then the corrected value is given by

$$T(E) = a\,T_u(E) + b(E)\,, \qquad \text{(VE1.1)}$$

in which energy dependences have been explicitly displayed.

Input for the normalization a and four specific backgrounds is specified in Card Set 6 of the PARameter file (page 122c). The four backgrounds are

$$\begin{aligned} b_1(E) &= B_a\,, \\ b_2(E) &= B_b/\sqrt{E}\,, \\ b_3(E) &= B_c\times\sqrt{E}\,, \\ \text{and}\quad b_4(E) &= B_d\times e^{-B_f/\sqrt{E}}\,. \end{aligned} \qquad \text{(VE1.2)}$$

With this format, the user provides one value (which may be zero) for each of the five background parameters B_a through B_f. It is not possible, however, to give *more* than one value for any of the backgrounds; hence one cannot, with this format, specify two exponential decay rates for the background.

A second, more general, format for background functions is given in Card Set 13 (page 122q). Again, there are four different types of background functions; however, unlike those given above, any number of each type may be included, so that the "actual" background is the sum of all such functions. Further, an energy range may be specified for each function. The functional forms for these backgrounds are, respectively, constant, exponential, power, and exponential of a logarithmic function. Explicitly,

$$\begin{aligned} b_1(E) &= A\,, \\ b_2(E) &= Ae^{-Bt}\,, \\ b_3(E) &= A\,t^{B}\,, \\ \text{and}\quad b_4(E) &= e^{A+Bt+C/\ln(t)}\,, \end{aligned} \qquad \text{(VE1.3)}$$

in which the time t is derived from the energy in the usual manner,

$$t = \sqrt{\frac{m L^2}{2E}} \quad , \qquad \text{(VE1.4)}$$

where L is the flight-path length. If the value for L is already given (e.g., for transmission data), that value can be used here. Otherwise, L can be specified along with the other parameters for these functions.

Because any of these parameters (excluding *Emin*, *Emax*, and L) can be varied, partial derivatives of the theoretical values T are required. These derivatives are found directly from Eqs. (VE1.1 through VE1.4) and are not listed explicitly here. Derivatives generated prior to these corrections (i.e., derivatives with respect to resonance parameters, broadening parameters, etc.) are also corrected by the normalization factor, as needed.

For examples of the use of normalization and/or background functions, the reader is referred to the test cases that are distributed with the SAMMY code. Test cases TR32 and TR45 (among others) include normalization and constant background on Card Set 6 of the PARameter file. Test case TR56 specifically addresses the use of more general background functions provided in Card Set 13 of the PARameter file.

V.F STELLAR AVERAGED CAPTURE CROSS SECTIONS

Stellar averaged capture cross sections may be generated for nuclear astrophysics applications. These are similar to the Maxwellian average used in reactor applications (see Sect. V.I on Integral Quantities), but defined in a somewhat different fashion. They are obtained from the stellar reaction rate formula [KW84],

$$\left\langle \sigma(E)\sqrt{E} \right\rangle_{kT} = \int_0^\infty \sigma_{capture}\ \sqrt{E}\ W(E,kT)\, dE \quad , \tag{VF.1}$$

where *W(E,kT)* is the Maxwellian weighting factor

$$W(E,kT) = \frac{2\sqrt{E}\ e^{-E/kT}}{\sqrt{\pi}\,(kT)^2} \tag{VF.2}$$

and the capture cross section $\sigma_{capture}$ is generated from the resonance parameters. The integration is performed numerically in SAMMY, using techniques similar to those described in Section IV.B for the broadening integrals.

Energies in the above equations are center-of-mass. The cross sections generated from resonance parameters are, however, expressed in terms of laboratory energy. The conversion from center-of-mass to laboratory is

$$E = \frac{M}{m+M}\ E_{lab} \tag{VF.3}$$

where m is the mass of the incident neutron and M is the mass of the target nucleus. The integration variable is changed from E to E_{lab} before the integral is evaluated.

The numerical integration technique is used to evaluate Eq. (VF.1) instead of the analytical approximation which may be more familiar to nuclear astrophysicists, because the assumptions underlying the analytical approximation are not always valid (see below). SAMMY does, however, calculate and print the approximate value in addition to the numerical result, and provides a comparison between the two. (In addition to printing these in the LPT file output, SAMMY also generates an output file SAM16.DAT which contains only the table of stellar-averages.)

The assumptions under which the analytical approximation is derived are the following: (1) The function $e^{-E/kT}$ is constant across the width of a resonance. (2) The neutron width Γ_n is constant across the width of a resonance. (3) The multilevel Breit-Wigner approximation provides an adequate description for the cross section. (4) The lower-energy limit may be extended from 0 to $-\infty$. Under these assumptions, the Maxwellian average has the approximate value

$$\left\langle \sigma(E)\sqrt{E} \right\rangle_{kT} \approx \frac{\pi^{3/2}}{m}\left(\frac{1}{kT}\right)^2 \sum_{\lambda} e^{-\frac{M}{m+M}\frac{E_\lambda}{kT}} \frac{2\,g_\lambda \Gamma_{\lambda n}\Gamma_{\lambda\gamma}}{\Gamma_\lambda} + \sqrt{\frac{E_{thermal}}{kT}}\,\sigma_{capture}(E_{thermal}) \quad , \tag{VF.4}$$

where the summation includes only those resonances which have positive energies, and the "thermal" energy is somewhat arbitrarily taken to be the lowest energy for which the differential cross sections are calculated. (This is sufficient, since results are the same so long as the energy is low enough that the energy-dependence is $1/V$, i.e., $1/\sqrt{E}$.)

To generate Maxwellian averages [both the numerically-integrated values of Eq. (VF.1) and the analytic approximation values of Eq. (VF.4)], include a line in the INPut file specifying one of the following two statements; note that these are treated identically within SAMMY:

```
MAXWELLIAN AVERAGED capture cross sections are wanted
STELLAR AVERAGED CAPture cross sections are wanted
```

It is also necessary to provide an additional input file, the MXW file, containing values for the temperatures at which the calculation is to be performed. See Section VI.H, page 130k, for details; also see Table VID.5 on page 130d for batch input.

There are several options in SAMMY for specifying the energy grid on which the numerical integration of Eq. (V.F.1) will take place. Because the precision with which the results are calculated may depend upon the method chosen, the user is encouraged to try different options to ensure that he is achieving the desired accuracy. The first option is to use an experimental (i.e. user-provided) grid; a better alternative is to begin with the experimental grid, but also specify

```
BROADENING IS WANTED
```

and give values for at least one broadening parameter. (This might be considered the "default," since this is what would apply if stellar averages were requested but no other thought was given to the specifics.) If the Doppler temperature is specified, it is used only to calculate an energy grid; the cross sections in the Maxwellian average are of course evaluated at zero temperature.

The purpose of specifying that broadening is wanted is to force SAMMY to choose a sufficiently dense auxiliary grid (see Section IV.B.1) to properly describe the structure in the cross section, and thus to ensure accurate integration. Additionally the user may wish to request extra points added between experimental points (see variable NXTRA in Card Set 2 of the INPut file, Table VIA.1).

Two other options permit SAMMY to choose the energy grid automatically. The first uses the (NJOY) reconstruct option via the command

```
RECONSTRUCT CROSS SEction from resonance parameters.
```

(This command can be used only with Reich-Moore approximation.). The other option (which can be used also with Breit-Wigner) begins with a uniformly-spaced grid, then adds points as needed to describe the structure. This option is invoked with the command

```
ARTIFICIAL ENERGY GRid is needed
```

The number of energy-points in the initial (uniformly spaced) grid is given by variable NEPNTS on Card Set 2 in the INPut file (Table VIA.1).

In all cases, the user specifies EMIN and EMAX as limits for the differential data. Within those energy limits, SAMMY will generate the capture cross section on the chosen energy grid and use those data points for the numerical integration process. External to those limits (i.e., below EMIN and above EMAX), SAMMY will extrapolate in an appropriate fashion in order to reach the integration limits (0 to ∞). SAMMY will issue warnings if the limits seem too confining (i.e., if the integrand does not approach zero at high energy).

Estimates of the covariance matrix for the stellar averaged capture cross section may be found by using default specifications for solving Bayes' equations (i.e. by not specifying

```
DO NOT SOLVE BAYES EQUATIONS
```

in the INPut file) and assigning uncertainties (and possibly correlations) to the flagged parameters. Those uncertainties will then be propagated through the averaging process, and the covariance matrix for the stellar averaged capture cross section will be generated. Caveat: Only those uncertainties included, either implicitly or explicitly, on the flagged parameters will contribute to the uncertainties on the averages. This may result in an underestimation of the uncertainties on the averages, since not all resonance parameter uncertainties can be included.

Often it is important to include values for the capture cross section at higher energies than those described by resonance parameters, i.e. in the unresolved resonance region. Currently the only way to accomplish this within SAMMY is to present this data as an ENDF file, and include the phrase

```
ADD CROSS SECTIONS From endf/b file 3
```

in the INPut file. SAMMY will ask for the name of this file immediately following the name of the MXW file (see Table VID.5 on page 130d). For the numerical integration results, the File-3 values are added directly to the resonance cross section before integration; in this case the differential data are still extrapolated to zero but the extrapolation beyond EMAX is based on the File-3 values. For the analytic approximation, the File-3 cross sections are integrated (numerically) separately and the results reported both separately and summed with the approximation results.

Test Case 51 (tr51) contains examples of the various options described above.

V.G RECONSTRUCTING POINT-WISE CROSS SECTIONS

SAMMY has two options for generating point-wise cross sections without requiring the user to provide an energy grid.

The first method, borrowed almost directly from the nuclear data processing code NJOY [RM82], uses a convergence algorithm to choose an energy grid sufficiently dense to properly define total, elastic, and capture cross sections, as well as fission if needed. The output ODF (plot) file SAMMY.ODF contains energies in Section 1, total cross section in Section 2, elastic cross section in Section 3, capture cross section in Section 4, and fission cross sections in Sections 5 & 6 if needed; these cross sections are unbroadened (zero temperature). To invoke this option, include the phrase

```
RECONSTRUCT CROSS Sections from resonance parameters
```

in Card Set 3 of the INPut file (see Section VI.A of this report). SAMMY will ask for the data file name, as always, but a dummy name may be given since that information is never used.

Caveat: The method described above makes use of the Reich-Moore approximation to R-Matrix theory. Thus it cannot be used with MLBW or SLBW resonance parameters.

The second option for generating point-wise cross sections without specifying an energy grid *a priori* makes use of SAMMY's ability to choose an auxiliary grid which properly defines the unbroadened cross section (see Section IV.B.1). The user must provide some kind of a "data file" but it need not necessarily be appropriate for the nuclide(s) being considered; it is used only as a starting point for the auxiliary grid. SAMMY first sets up a grid of NEPNTS from EMIN to EMAX; NEPNTS is specified on Card Set 2 of the INPut file (see Table VIA.1). This grid is evenly-spaced in velocity-space (i.e. in the square root of energy). SAMMY then chooses additional points for the auxiliary grid as though broadening were to occur.

To invoke this option include the phrases

```
ARTIFICIAL ENERGY GRid is needed
```

and

```
PUT UNBROADENED CROSs sections into odf file
```

in the INPut file. An output ODF file SAMXAC.ODF contains energies in Section 1 and cross section in Section 2. Unlike the RECONSTRUCT method of generating an energy grid, this method evaluates only the one type of cross section specified in the INPut file. Also unlike the first method, any of the several R-matrix approximations may be used, as specified in the INPut file.

Examples of reconstructing point-wise cross sections using both of these methods can be found in several Test Cases. See, specifically, tr37 for "pure" reconstruction, and tr42 and tr49 for reconstruction followed by computation of stellar (Maxwellian) averages.

V. J UNRESOLVED RESONANCE REGION

As a first step towards expansion into the unresolved resonance region, Fritz Fröhner's code FITACS [FF89] has been obtained and inserted into SAMMY. FITACS uses Hauser-Feshbach theory with width fluctuations. The adjustable parameters are strength functions, distant-level parameters, average radiation widths (at $E = 0$), and average fission widths (at $E = 0$). The energy dependence of the radiation widths is specified via the giant dipole model, of the fission widths via Hill-Wheeler fission barrier transmission coefficients, and of the mean level spacing for s-waves via the Gilbert-Cameron composite formula. Mean spacings for $l > 0$ are given via Bethe formula. Moldauer's prescription is used for partial cross sections. Details of the theory are presented in Section V.J.1.

Initially (for release M2 of the code), FITACS was incorporated into SAMMY (as segments SAMFFF and SAMACS) in a limited fashion only: Internal changes were made, to be consistent with SAMMY notation and to use dynamic dimensioning of arrays. The $M + W$ version of Bayes' method has replaced the fitting procedure used in FITACS. Calculation of penetrabilities was extended to all l values (FITACS had used only s, p, d, and f-waves). The output included files from which plots can be made. Results are reported in SAMMY.PAR in the same format as is used in the input file (as well as in more human-legible fashion in SAMMY.LPT). No other significant changes were made in the FITACS input, method of calculation, or output.

For release M5 (and subsequent releases), the following modifications and improvements have been made:

- Partial derivatives with respect to varied parameters are now calculated exactly rather than approximately.
- A more efficient integration routine has been written for the Dresner integral.
- It is possible to include (and vary, if desired) a normalization for each data set.
- There is no limit on number or type of experimental data sets. Data may be kept in separate files rather than appended to the parameter file.
- The output has been modified to conform more closely to SAMMY conventions.

One additional change is planned for the future: a link between the resolved-resonance parameters and those for the unresolved region is needed, in order to provide more consistent evaluated cross sections.

Input for analysis of data in the unresolved-resonance region is described in Section V.J.2.

Note that, for the unresolved-resonance region, the fit to all data sets is performed simultaneously. This is in contrast to the usual SAMMY treatment for the resolved-resonance region, for which the fit is sequential (output PARameter and COVariance files from the fit to one data set are used as input to the fit to another data set).

V. J.1 Equations for Unresolved Resonance Region

In this section are presented the formulae for cross sections in the unresolved-resonance region, as implemented in SAMMY. The implementation is a modified form of that provided by Fritz Fröhner in his FITACS code [FF89]. (Please note that any mistakes in these formulae are attributable only to the author of this manual, not to Fröhner. The author is indebted to Herve Derrien for significant contributions both to the development of the code and to the composition of this section of the manual.)

The average total cross section, for a given spin and parity and incident channel c, may be written according to Hauser-Feshbach theory as

$$<\sigma_c> = \frac{2\pi g_c}{k_c^2}\,(1 - \mathrm{Re}<S_{cc}>) \quad , \tag{VJ1.1}$$

where, as usual, g_c is the spin factor and k_c is the center-of-mass momentum. The average scattering matrix $<S>$ is given by

$$<S_{cc}> = e^{-2i\varphi_c}\,\frac{1 - <R_{cc}> L_c^{0*}}{1 - <R_{cc}> L_c^{0}} \quad , \tag{VJ1.2}$$

and the average R-matrix can be written in the form

$$<R_{cc}> = R_c^{\infty} + i\pi s_c \quad , \tag{VJ1.3}$$

with parameters defined as follows:

φ_c = hard-sphere scattering phase;

R_c^{∞} = distant-level parameter (an input quantity);

s_c = pole strength, equal to $S_c\sqrt{E}\,/\,2\,k_c\,a$, where S_c is the strength function (an input quantity) and a is the R-matrix matching radius (also an input quantity);

L_c^0 = $(S-B) - iP$ (See Sect. III.A), with boundary condition B chosen such that $S - B = 0$.

The (non-elastic) partial cross sections are given by Moldauer's prescription [PM80], which may be written in terms of "transmission coefficients" T_x as

$$<\sigma_{ab}> = \frac{2\pi g_a}{k_a^2}\,\frac{T_a T_b}{T}\int_0^{\infty} dt\; e^{-tT_\gamma/T}\prod_{c\in\gamma}\left(1 + \frac{2}{\nu_c}\frac{T_c}{T}t\right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \tag{VJ1.4}$$

[A derivation of this expression, including the assumptions under which it is derived, is provided in Section V.J.1.a.] Here a represents the incident channel and b the exit channel; ν_c and T_c represent the degrees of freedom (multiplicity) and transmission coefficient respectively for channel c. Subscript γ refers to photon channels. T is defined as the sum over all channels,

$$T = \sum_c T_c \qquad \text{(VJ1.5)}$$

The transmission coefficient for neutron channels is given by

$$T_c = 1 - |\langle S_{cc} \rangle|^2 = \frac{4\pi P_c s_c}{1 - \langle R_{cc} \rangle L_c} \quad , \qquad \text{(VJ1.6)}$$

where c is an incident channel, P and L are as defined in Section III.A, and the other quantities are given above. For photon and fission channels, the transmission coefficients for spin J are

$$T_\gamma = 2\pi \langle \Gamma_\gamma \rangle / D_J \quad \text{and} \quad T_f = 2\pi \langle \Gamma_f \rangle / D_J \quad , \qquad \text{(VJ1.7)}$$

in which D_J is the mean level spacing for levels with this spin.

The J-dependence of the mean level spacing is set in SAMMY/FITACS via the Bethe formula [e.g., FF83],

$$\left(D_J(E)\right)^{-1} = \left(d(E)\right)^{-1} \left\{ \exp\left[\frac{-J^2}{2\left(\sigma(E)\right)^2}\right] - \exp\left[-\frac{(J+1)^2}{2\left(\sigma(E)\right)^2}\right] \right\} \quad , \qquad \text{(VJ1.8)}$$

where d is independent of J, and σ is the spin cutoff parameter. The spin cutoff parameter is related to the level density parameter a and the energy E by the formula

$$\sigma = \sqrt{4a(E + BE - PE)} \quad , \qquad \text{(VJ1.9)}$$

in which BE represents the neutron binding energy (an input parameter) and PE the pairing energy (also an input parameter). The value for a is determined from the input quantity D, which is the mean level spacing of the $l = 0$ resonances at $E = 0$; note that D includes both $J = I - i$ and $J = I + i$, where I is the spin of the target nucleus and $i = ½$ is the spin of the neutron. An expression for the inverse of D can be found from Eq. (VJ1.8) to be

$$\begin{aligned} D^{-1} &= \sum_{J \text{ with } l=0} \left(D_J(E=0)\right)^{-1} \\ &= \left(d(0)\right)^{-1} \left\{ \exp\left[\frac{-(I-1/2)^2}{2\sigma^2}\right] - \exp\left[-\frac{(I+3/2)^2}{2\sigma^2}\right] \right\} \quad ; \end{aligned} \qquad \text{(VJ1.10)}$$

this expression is used to determine the value of σ^2 and hence of the level density parameter a.

The energy dependence of the mean level spacing is calculated with the Gilbert-Cameron composite formula [AG65]. Let E_x represent the excitation energy of the compound nucleus; this energy is equal to the sum of the incident neutron energy E and the neutron binding energy BE (which is an input quantity). That is to say,

$$E_x = E + BE \quad . \tag{VJ1.11}$$

The energy dependence for low excitation energies ($E_x \le E_0$), where E_0 is a matching energy, is given by the constant-temperature formula

$$D^{-1} \propto C_3 \frac{\exp\left(C_2\sqrt{E_0 - PE}\right)}{(E_0 - PE)^{3/2}} \exp\left[\frac{E_x - E_0}{2}\left(\frac{C_2}{\sqrt{E_0 - PE}} - \frac{3}{E_0 - PE}\right)\right] \quad . \tag{VJ1.12}$$

In the code, the matching energy E_0 is set at (5/2 + 150/(N+Z+1)) MeV with (N+Z) being the mass number for the target nucleus. Values of the constants C_2 and C_3 are given by

$$C_2 = \sqrt{4a} \quad \text{and} \quad C_3 = \frac{1}{12\sqrt{2aq}} \tag{VJ1.13}$$

with q defined as

$$q = (0.608)(0.240)(A+1)^{2/3} \tag{VJ1.14}$$

where $A = N + Z$ is the mass number for the target nucleus.

At higher energies ($E_x \ge E_0$), the energy dependence of the mean level spacing is calculated via the Fermi-Gas formula

$$D^{-1} \propto C_3 \frac{\exp\left(C_2\sqrt{E_x - PE}\right)}{(E_x - PE)^{3/2}} \quad . \tag{VJ1.15}$$

Note that the two formulae agree at the matching energy (i.e., at $E_x = E_0$).

Radiation widths $\langle\Gamma_\gamma\rangle$ are assumed to depend only on parity π and on E. The energy dependence is calculated with the giant dipole resonance model.

Fission widths $\langle\Gamma_f\rangle$ may vary with spin as well as parity and incident neutron energy E. Energy dependence is calculated with the Hill-Wheeler fission barrier transmission coefficients [DH53]. For a given $J\pi$ the energy dependence of the fission widths is taken to be

$$<\Gamma_f(E)> = <\Gamma_f(0)> \frac{1 + \exp\left(E_{HW} / W_{HW}\right)}{1 + \exp\left(-(E - E_{HW}) / W_{HW}\right)} \quad , \qquad \text{(VJ1.16)}$$

where the Hill-Wheeler threshold energy E_{HW} and the Hill-Wheeler threshold width W_{HW} are input quantities. This equation may be written in more "standard" notation as

$$<\Gamma_f(E)> = <\Gamma_f(0)> \frac{1 + \exp\left(2\pi(E_f - BE) / \hbar\omega\right)}{1 + \exp\left(-2\pi\left(E_x - (E_f - BE)\right) / \hbar\omega\right)} \quad , \qquad \text{(VJ1.17)}$$

where, as above, E_x is the excitation energy of the neutron and BE is the binding energy. Also, E_f is the fission barrier height, and $\hbar\omega$ the width of the fission barrier.

Finally, a few words regarding the derivation of Eq. (VJ1.4) are warrented. That derivation is based on several assumptions: (1) Single-level Breit-Wigner is an adequate description of the cross section (i.e., resonances are well separated). (2) Widths obey the Porter-Thomas distribution (chi-squared with one degree of freedom); averages are therefore weighted with this distribution. (3) The average of products can be written as the product of averages. (4) Channels with the same transmission coefficients may be combined by introducing multiplicities.

The integral of Eq. (VJ1.4) is described by Fröhner as the "width fluctuation correction or Dresner factor." One (relatively modest) difference between SAMMY and the original FITACS coding is the algorithm for calculating the Dresner integral; in SAMMY, the coding has been refined to increase both speed and accuracy of calculation by using a non-uniform grid designed specifically for this task.

V.J.1.a Derivation of non-elastic average cross section

Derivations shown in this section are based on (1) notes provided by Fritz Fröhner [FF99] and (2) discussions with Herve Derrien [HD00]. Any errors in these pages are the responsibility of the SAMMY author alone.

The single-level Breit-Wigner formula for the cross section at energy E, Eq. (IIIC1.5), for the transition from channel *a* to channel *b* (where $a \neq b$), takes the form

$$\sigma_{ab} = \frac{\pi g_a}{k_a^2} \sum_{\lambda} \frac{\Gamma_{\lambda a}\Gamma_{\lambda b}}{(E-E_\lambda)^2 + (\Gamma_\lambda/2)^2} \quad ; \qquad \text{(VJ1a.1)}$$

this expression forms the basis for the calculation of the average cross section. The corresponding average cross section in an energy interval containing a large number of resonances may be written as

$$<\sigma_{ab}> = \frac{\pi g_a}{k_a^2}\, 2\pi\rho_a \left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle \quad , \qquad \text{(VJ1a.2)}$$

where ρ is the level density, and the brackets refer to averages. (Note that the subscript λ has been dropped for simplicity's sake.) The calculation of the average quantity

$$\left\langle \frac{\Gamma_{\lambda a}\Gamma_{\lambda b}}{\Gamma_\lambda} \right\rangle$$

is not straightforward, since the known parameters are $\langle \Gamma_{\lambda a} \rangle$ and $\langle \Gamma_{\lambda b} \rangle$ (from the statistical properties of the resonance parameters). One has to take into account the fluctuations of the partial widths of the resonances from the chi-squared distribution of the parameters.

A method of calculating the average

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle$$

from the known entities

$$\frac{\langle \Gamma_a \rangle \langle \Gamma_b \rangle}{\langle \Gamma \rangle}$$

was proposed by Dresner [FF99]. He suggested making the substitution

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \left\langle \frac{\Gamma_a \Gamma_b}{\sum_{\text{all } c} \Gamma_c} \right\rangle = \left\langle \Gamma_a \Gamma_b \int_0^\infty dq\, \exp\left(-q \sum_{\text{all } c} \Gamma_c\right) \right\rangle \quad , \qquad \text{(VJ1a.3)}$$

which follows from the identity

$$\int_0^\infty dq\, e^{-qQ} = \frac{1}{Q}\int_0^\infty dy\, e^{-y} = \frac{1}{Q} \quad . \tag{VJ1a.4}$$

The product of partial widths in Eq. (VJ1a.3) can be rearranged as

$$\left\langle \Gamma_a \Gamma_b \int_0^\infty dq \exp\left(-q\sum_{\text{all } c}\Gamma_c\right)\right\rangle = \left\langle \int_0^\infty dq\, \Gamma_a e^{-q\Gamma_a}\, \Gamma_b e^{-q\Gamma_b} \prod_{c\neq a,b} e^{-q\,\Gamma_c}\right\rangle \quad .$$

Because the channels a, b, and c are independent, the average of the product is equal to the product of the averages. Likewise integration over q is independent of the averaging process; hence Eq. (VJ1a.3) can be rewritten as

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma}\right\rangle = \int_0^\infty dq \left\langle \Gamma_a e^{-q\Gamma_a}\right\rangle \left\langle \Gamma_b e^{-q\Gamma_b}\right\rangle \prod_{c\neq a,b}\left\langle e^{-q\,\Gamma_c}\right\rangle \quad . \tag{VJ1a.5}$$

One assumes the partial widths obey a chi-squared distribution with ν degrees of freedom, which has the form

$$\rho(x,\nu)\,dx = \left[\Gamma\left(\frac{\nu}{2}\right)\right]^{-1}\left(\frac{\nu x}{2}\right)^{\nu/2-1} e^{-\nu x/2}\,\frac{\nu}{2}\,dx \quad , \tag{VJ1a.6}$$

where Γ refers to the Gamma-function. Note that ν = 1 corresponds to the Porter-Thomas distribution for a single neutron channel; ν = 2 corresponds to two channels. For fission, the value of ν depends on the number of open or partially open fission channels; ν_f is an input parameter in SAMMY (and in FITACS).

Applying this distribution to the average quantity needed in Eq. (VJ1a.5), with $x = \Gamma_c/\langle\Gamma_c\rangle$, gives

$$\left\langle e^{-q\,\Gamma_c}\right\rangle = \frac{1}{\Gamma(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}-1}\int_0^\infty e^{-q\langle\Gamma_c\rangle x}\, x^{\frac{\nu}{2}-1}\, e^{-\nu x/2}\,\frac{\nu}{2}\,dx \quad , \tag{VJ1a.7}$$

which can be rewritten into the form

$$\begin{aligned}\left\langle e^{-q\,\Gamma_c}\right\rangle &= \frac{1}{\Gamma(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}\left(\frac{\nu}{2}+q\langle\Gamma_c\rangle\right)^{-\frac{\nu}{2}}\int_0^\infty e^{-w}\, w^{\frac{\nu}{2}-1}\,dw \\ &= \frac{1}{\Gamma(\nu/2)}\left(1+\frac{2}{\nu}q\langle\Gamma_c\rangle\right)^{-\frac{\nu}{2}}\Gamma(\nu/2) \\ &= \left(1+\frac{2}{\nu}q\langle\Gamma_c\rangle\right)^{-\frac{\nu}{2}} \quad .\end{aligned} \tag{VJ1a.8}$$

Hence Eq. (VJ1a.5) can be expressed as

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \left\langle \Gamma_a \right\rangle \left\langle \Gamma_b \right\rangle \int_0^\infty dq \prod_c \left(1 + \frac{2}{\nu_c} \left\langle \Gamma_c \right\rangle q \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} , \qquad \text{(VJ1a.9)}$$

in which the correspondence of ν with channel c is made explicit by the addition of the subscript. Making a change of variable from q to $t = <\Gamma> q$ gives

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \frac{<\Gamma_a><\Gamma_b>}{<\Gamma>} \int_0^\infty dt \prod_c \left(1 + \frac{2}{\nu_c} \frac{<\Gamma_c>}{<\Gamma>} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \qquad \text{(VJ1a.10)}$$

The "transmission coefficients" are related to the widths by

$$T_c = 2\pi \rho_c <\Gamma_c> \qquad \text{(VJ1a.11)}$$

Note the equality of the level densities, $\rho_a = \rho_b = \rho_c = \rho_J$, since all refer to the same spin and parity. Hence Eq. (VJ1a.10) can be rewritten as

$$2\pi \rho_a \left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \frac{T_a T_b}{T} \int_0^\infty dt \prod_c \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} , \qquad \text{(VJ1a.12)}$$

so that the cross section can be expressed as

$$<\sigma_{ab}> = \frac{2\pi g_a}{k_a^2} \frac{T_a T_b}{T} \int_0^\infty dt \prod_c \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} . \qquad \text{(VJ1a.13)}$$

For photon channels, the limit of non-fluctuating radiation widths, $\nu_{c=\gamma} \to \infty$ gives

$$\lim_{\nu_\gamma \to \infty} \left(1 + \frac{2}{\nu_\gamma} \frac{T_\gamma}{T} t \right)^{-\frac{\nu_\gamma}{2}} \to e^{-t T_\gamma / T} \qquad \text{(VJ1a.14)}$$

Therefore our expression for the cross section, Eq. (VJ1a.13), takes the form

$$<\sigma_{ab}> = \frac{2\pi g_a}{k_a^2} \frac{T_a T_b}{T} \int_0^\infty dt\, e^{-t T_\gamma / T} \prod_{c \in \gamma} \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} , \qquad \text{(VJ1a.15)}$$

which is equivalent to Eq. (VJ1.4). QED.

Evaluation of this expression for the average cross section in SAMMY (and in FITACS) assumes further simplification: first, we make the change of variable from t to $q = t\,T_\gamma / T$,

$$<\sigma_{ab}> = \frac{2\pi g_a}{k_a^2}\,\frac{T_a T_b}{T_\gamma}\int_0^\infty dq\; e^{-q}\prod_{c\in\gamma}\left(1+\frac{2}{\nu_c}\frac{T_c}{T_\gamma}q\right)^{-\nu_c/2-\delta_{ac}-\delta_{bc}} \qquad \text{(VJ1a.16)}$$

Second, we then change variable from q to $u = e^{-q}$ to obtain

$$<\sigma_{ab}> = \frac{2\pi g_a}{k_a^2}\,\frac{T_a T_b}{T_\gamma}\int_0^1 du\prod_{c\in\gamma}\left(1+\frac{2}{\nu_c}\frac{T_c}{T_\gamma}\ln u\right)^{-\nu_c/2-\delta_{ac}-\delta_{bc}} \qquad \text{(VJ1a.17)}$$

Next, define parameters b_c via

$$b_c = \frac{2}{\nu_c}\frac{T_c}{T_\gamma}\;, \qquad \text{(VJ1a.18)}$$

and substitute into Eq. (VJ1a.16) to give

$$<\sigma_{nx}> = \frac{\pi g}{k^2}\,T_\gamma\sum_{\alpha|n}\sum_{\alpha'|x}\nu_\alpha b_\alpha\,\nu_{\alpha'}b_{\alpha'}\int_0^1 du\prod_{\alpha''\in\gamma}\left(1-b_{\alpha''}\ln u\right)^{-\nu_{\alpha''}/2-\delta_{\alpha\alpha''}-\delta_{\alpha'\alpha''}}$$

$$= \frac{\pi g}{k^2}\,T_\gamma\,Q_{nx} \qquad \text{(VJ1a.19)}$$

where Q is defined as

$$Q_{nx} = \sum_{\alpha|n}\sum_{\alpha'|x}\nu_\alpha b_\alpha\,\nu_{\alpha'}\,b_{\alpha'}\,I_{\alpha\alpha'} \qquad \text{(VJ1a.20)}$$

with

$$I_{\alpha\alpha'} = \int_0^1 du\prod_{\alpha''\in\gamma}\left(1-b_{\alpha''}\ln u\right)^{-\nu_{\alpha''}/2-\delta_{\alpha\alpha''}-\delta_{\alpha'\alpha''}} \qquad \text{(VJ1a.21)}$$

The expression for $I_{\alpha\alpha'}$ is denoted the "Dresner integral". Evaluation of this integral is accomplished in SAMMY by (1) choosing a grid for u in which the spacing between points increases as the integrand flattens and (2) using a quadratic quadrature scheme. This integration scheme was tested with a wide range of plausible values for b's and ν's, comparing results for various values of N (where N is the number of points in the u-grid). Results were good to six digits of accuracy, for all tested values of b's and ν's, using as few as 201 points in the grid.

V. J.2 Input for Analysis of Data in Unresolved-resonance Region

Two or more input files are required for the use of this option. The first is the SAMMY INPut file, which contains three lines only: Card Set 1 of Table VIA.1 (the title line), Card Set 2 (nuclide name, atomic weight, and energy range), and (at least) one line for Card Set 3 (alphanumeric information). The alphanumeric line contains the phrase UNRESOLVED RESONANCE REGION. A second alphanumeric line may be included if desired; this line reads EXPERIMENTAL DATA ARE IN SEPARATE FILES.

The second file may be exactly the same as Fröhner's original FITACS file (which includes both parameters and data). To inform the code that a parameter is to be varied, FITACS assumes that, if the uncertainty is given as zero for a given parameter, then that parameter is not varied. (Hence there is no means of provide a default value for uncertainty). This procedure is in contrast with the usual SAMMY procedure of assigning a value (generally, 1) to a flag for each varied parameter. [In the future, the formats for input to the FITACS portion of SAMMY will perhaps be modified to conform to SAMMY standards.] Currently all numbers, both integer and real, are specified with F10 formats. See Table VJ.2.1 for the input to this ACS file.

To run this option (using the original FITACS input), the user should specify the two file names, the INPut file on one line and the ACS file on the next. No other input is required.

SAMMY now permits two types of modifications to the ACS file. First, each data set (corresponding to lines 16-21 in Table V.J.2.1) may be kept in a separate file rather than included as a portion of the ACS file. To use this option, include the line EXPERIMENTAL DATA ARE IN SEPARATE FILES in the INPut file, and list the files names following the INPut and ACS file names in the on-screen (or batch) input stream. (Also of course omit lines 16-22 from the ACS file.)

Secondly, normalizations can now be included (and varied) for each data set. That is, the theoretical calculation of the cross section is modified by

$$Theory = norm \times \sigma_{calculated}$$

where *norm* is given by the formula

$$norm = a + b\,E^{c}$$

and a, b, and c are input parameters, specified in the ACS file. Note that one set of values for a, b, and c is given for each data set.

Test case tr73 gives sample input and output for use of this option.

Table VJ2.1. Input for ACS file for treatment of the unresolved resonance region

Line No.	Description
1 - 4	First four lines are alphanumeric title
5	Number of iterations, fitting tolerance (essentially, delta chi-squared). Note that integers are to be specified as real numbers. All formats are F10
6	Mass in amu, radius in Fermi (or use default), neutron binding energy in MeV, pairing energy *PE* in MeV. Again, formats are F10
7,8,...	Center-of-mass excitation energy, spin, and parity for the *n*th target level (beginning with ground state)
9	(Blank)
10	Strength function S_c, uncertainty, distant-level parameter R_c^{∞}, uncertainty, radiation width $<\Gamma_\gamma>$ in eV, uncertainty, mean level spacing D in eV for $l = 0$
11	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 1$
12	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 2$
13, 14, ...	As above, for higher l values as needed
15	(Blank)
16	Average fission width $<\Gamma_f>$ (eV), degree of freedom ν_f for fission width distribution, Hill-Wheeler threshold energy E_{HW}, HW threshold width W_{HW}, uncertainty on the average fission width, for lowest J value.
17, 18, ...	Repeat card 16 for each possible value of J.
19	(Blank)
20	Type of cross-section data (TOTAl, CAPTure, FISSion, or INELastic)
21	Uncertainties are RELAtive or ABSOlute
22, ...	Energy, cross section, uncertainty (Note: if RELAtive then need specify only for first data point, rest are assumed to be the same)
23	(Blank)
24, ...	Repeat 18 to 21 as many times as needed, in any order
25	The single word "NORMALIZATION" in all capital letters or all lower case
26	Type of cross section, normalization parameters a, Δa, b, Δb, c, Δc, where the normalization for this data set is given by $norm = a + b E^c$
27, etc.	Repeat once for each data set. Note that normalizations must appear in the same order in which the data sets appear. SAMMY will check to be sure the data types are consistent

V. L INDIVIDUAL REACTION TYPES

Earlier versions of SAMMY permitted users to specify "inelastic", "fission", and "reaction" data, and indeed such data types could be calculated in the code. The tacit assumption, however, was that the exit channels included only channels which are relevant to the type of data being used. If, for example, three exit channels were specified as (1) inelastic, (2) first fission channel, and (3) second fission channel, then any calculation for "inelastic", "fission", or "reaction" data types would automatically include all three exit channels in the final state.

Hence, in earlier versions of SAMMY, true inelastic cross sections (for example) would be calculated only if all of the following conditions were met:

1. Either "inelastic", "fission", or "reaction" was specified as the data type in the INPut file, Card Set 8; and
2. The exit channel description was appropriate for inelastic channels: The INPut file noted that penetrabilities were to be calculated (LPENT = 1 on Card 2 of "Alternate to Card Set 10") and also provided a non-zero value for the excitation energy; and
3. No fission channel (or other exit channel) was defined in the INPut file (and PARameter file).

Beginning with release M5 of the SAMMY code, it is now possible to include a subset of the exit channels in the outgoing final state. The third condition in the list above is no longer necessary, but is replaced by another (less restrictive) condition:

3. Exit channels which are not inelastic channels have a flag ("1" in Column 18 of Card 2 of "Alternate to Card Set 10 of the INPut file) denoting that this channel does not contribute to the final state.

See test case TR93 for an example which includes two reactions, the first being (n,α) and the second (n,n′).

VI. INPUT TO SAMMY

Input to SAMMY consists of three or more files, which may be user-generated or (sometimes) produced by earlier SAMMY runs. These files are summarized in Table VI.1 and described in detail in the sections listed. Test case numbers (see Sect. XI.D) are given for those files which are infrequently used.

Table VI.1. SAMMY input files

Description	Contents	Where details may be found	Used in which test case
Batch file	Interactive or batch input to SAMMY; file names, energy ranges	Section VI.D	
INPut file	Details about the interaction being studied; SAMMY control information	Section VI.A Tables VIA.1 & 2	
PARameter file	Initial values for resonance and other parameters, flags defining which are to be varied, uncertainty information	Section VI.B Table VIB.1	
DATa file	Experimental data, including energy, cross section (or transmission, e.g.), and uncertainty	Section VI.C.1 Table VIC1.1	
COVariance file	Covariance matrix for the parameters as output by an earlier SAMMY run	Section VII.B	
DCV (Data CoVariance)	Covariance information for the data	Section VI.C.2	tr7
IDC (Implicit Data Covariance)	Information on data-reduction parameters to be used to generate implicit data covariance matrix	Section VI.C.3	tr70
AVG file or BON file	Information needed by SAMMY in order to produce energy-averaged or Bondarenko-averaged cross sections	Section VI.E	tr14, tr83, tr84, tr85

Table VI.I (continued)

Description	Contents	Where details may be found	Used in which test case
NTG file	Integral data file	Section VI.I	tr69, tr77
NDF input file	Information needed by SAMMY in order to generate an output file in ENDF-6 File 2 format	Section VI.F	tr23
ENDF resonance parameter file	File 2 from ENDF, to be used instead of the usual SAMMY PARameter file (and for part of the SAMMY INPut file)	Section VI.G	tr50
ENDF File 3	Smooth cross sections to be added to the cross section calculated from resonance parameters, for use in calculating the stellar (Maxwellian) averages	Section V.F	tr51
MXW file	Temperatures at which the stellar (Maxwellian) averages are to be evaluated	Sections V.F and VI.H	tr42, tr49, tr51
SSM file	Edge-effects corrections to single-scattering correction for capture cross sections (file is generated by a previous SAMMY run)	Section III.F	tr39
ACS file	Input information for Unresolved Resonance Region	Section V.J	tr73, tr88
THN file	Directions for thinning data	Section VIII.G	tr72

VI.A THE INPut FILE

Table VIA.1 gives details about the information provided to SAMMY via the INPut file.

Card Set 1 of the table contains a title, which is reproduced in the output LPT file (See Section VII.A).

Card Set 2 contains miscellaneous information, including the mass of the sample, the energy range, a flag to indicate how many iterations of Bayes' equations are to be run. Some of the information given here may be input elsewhere, in which case numbers given here are ignored.

The user specifies control options via Card Set 3, which contains statements (in English) regarding the manner in which SAMMY is to proceed for this analysis. Valid control statements are given in Table VIA.2; any of these statements may be used in any order in Card Set 3. (In the case of a conflict between two statements, the later command is used.) Note that SAMMY does not understand misspellings! Instead, SAMMY will print an error message in the LPT file and proceed to ignore the statement. Control statements may be either capital letters or lowercase, but must be entirely one or the other on any given statement; that is, do not mix lowercase and capitals on the same line.

Card Set 4 is blank, terminating Card Set 3.

Card Sets 5 and 6 describe the input for Doppler- and resolution-broadening (See Section IV). Card Set 7 gives matching radius for the R-matrix formalism, sample thickness, and various other parameters. Values for many of these parameters may, however, be superseded by values specified in the PARameter file (See Section VI.B).

Card Set 8 specifies the type of data to be analyzed (e.g., capture cross section, transmission). When the data are angular distributions, angles are specified here.

Quantum numbers for the sample nucleus are specified in Card Set 9, though values given here may be overwritten by values given in "Alternative to Card Set 10."

Card Set 10 describes quantum numbers for the various spin groups. NOTE: The "Alternative to Card Set 10" is now the preferred method for inputting these quantum numbers, because in this format all spins, masses, etc. (e.g., of minor isotopes) may be given explicitly.

Card Set 11 is needed only when analyzing capture cross sections using self-shielding and multiple-scattering corrections. Dimensions of the sample, and interpolation and integration parameters, are specified in this Card Set.

Card Sets 12 (Oak Ridge Resolution Function) and 13 (RPI Resolution Function) are respectively equivalent to Card Sets 9 and 14 of the PARameter file, except that parameters cannot be varied when they appear in the INPut file.

Table VIA.1 Format of the INPut File

Note: All integer formats (e.g., I2, I5) require that the numbers be in the right-most columns

Card set	Number of cards in this set	Which card is shown here	Col-umn	Variable	For-mat	Meaning (units)	Range of values	Notes
1	1	1	1-80	TITLE	16A5			
2	1	1	1-10	ELMNT	A10	Sample element's name		
			11-20	AW	F10.1	Atomic weight (amu)		
			21-30	EMIN	F10.1	Minimum energy for this data set (eV)		EMIN & EMAX will be ignored here if they are given in the BATch file (See Section VI.D)
			31-40	EMAX	F10.1	Maximum energy (eV)		
			41-45	NEPNTS	I5	Maximum number of points to be analyzed at one time (default = 500, but see Note) or: number of points to be used in generating artificial energy grid (default = 10001)		NEPNTS is the number of data points to be included in each region when "DIVIDE DATA INTO REGions" is specified in Card Set 3. (See Section V.G; *use of this option is discouraged.*)
			49-50	ITMAX	I2	Number of iterations (default = 2)		
			51-52	ICORR	I2	Correlations smaller than this value (divided by 100) are not to be printed	$0 \leq$ ICORR ≤ 100 Default = 50	This value is ignored unless the phrase "DO NOT PRINT SMALL Correlation coefficients" occurs in Card Set 3
			53-55	NXTRA	I3	Number of extra points to be added between each pair of data points for the auxiliary energy grid	$0 \leq$ NXTRA ≤ 999 Default = 0	The minimum number of points in the auxiliary grid is (NXTRA+1) × NDAT, where NDAT is the number of points in the data grid

Table VIA.1 (continued)

Card set	Number of cards	Which card	Column	Variable	For-mat	Meaning (units)	Range of values	Notes
2, cont.	1	1, cont.	56-57	IPTDOP	I2	Number of points to be added to auxiliary energy grid in the neighborhood of small resonances	0≤ IPTDOP≤ 21 Default = 9	See Section IV.B.1
			59-60	IPTWID	I2	Determines the number of points to be added to auxiliary grid in tails of small resonances	-1≤ IPTWID≤ 6 Default = 5	
			61-70	IXXCHN	I10	Number of channels in ODF-type data file to be ignored, or, if MATNUM ≠ 0, IXXCHN = ZA for ENDF file		
			71-72	NDIGIT	I2	Number of digits for concise format	1 to 6	See Sect VII.E for details
			73-74	IDROPP	I2	Drop Correlations smaller than this %	1 to 99	
			75-80	MATNUM	I6	ENDF Material Number		
3	As many as needed		1-20	WHAT	4A5	Alphanumeric information concerning program options	See Table VIA.2	
4	1	1	blank					
5	0 or 1	1	1-10	TEMP	F10.1	Effective temperature of the sample (K)	(Zero for no Doppler broadening)	This Card Set is omitted if "BROADENING IS NOT Wanted" is specified in Card Set 3. If Card Set 4 appears in the PARameter file (see Table VIB.1), all values given here (in the INPut file) in Card Set 5 will be ignored, except for DIST. See Sect. IV.A.2.a
			11-20	DIST	F10.1	Flight path length (m)		
			21-30	DELTAL	F10.1	That portion of the resolution function width attributed to the flight path length (m)		

Table VIA.1. Continued

Card Set	Number of cards	Which card	Col-umn	Variable	Format	Meaning (units)	Range of Values	Notes
5, cont.	0 or 1	1, cont.	31-40	DELTAE	F10.1	E-folding width of exponential resolution function (μs)	(0 for pure Gaussian resolution function)	See Section IV.A.2.b. If the card "EXPONENTIAL FOLDING width is energy-dependent" is included in the INPut file, the value given here is used for DELTAE at 100 eV; at other energies, the value is given by Eq.(IVA2b.6) on page 69.
			41-50	DELTAG	F10.1	FWHM (μs) of Gaussian resolution function representing the burst width	(0 for pure exponential resolution function)	See Section IV.A.2.a, Eq. (IVA2a.13 and .15). If negative, channel widths are also included, in Card Set 6.
			51-60	DELTTT	F10.1	Approximate step size for Effective Temperature when using Leal-Hwang method of Doppler broadening (K)	> 0 default = 5.0	See Section IV.D.
			61-70	ELOWBR	F10.1	Energy below which no broadening is wanted (eV)	default = 0.0	
6	0 or 2	1	1-10	DELTAB	F10.1	Minimum channel width for interval from EMIN to EMAX (μs)		This Card Set is included only if DELTAG< 0 in Card Set 5
			11-15	NCF	I5	Number of crunch boundaries (energy intervals)		
		2	1-10 11-20 etc.	(BCF(I), CF(I), I=1,NCF)	8F10.1	Crunch boundaries, read in order of increasing energy (eV). Crunch factors (integer units of DELTAB)		BCF(I) = maximum energy for this crunch factor; CF(I) = crunch factor; i.e. the value of Δt_c to be used in the energy range BCF(I-1)<E<BCF(I) is CF(I)×DELTAB. See Eq. (IVA2a.7) and following.

Table VIA.1. Continued

Card Set	Number of cards	Which card	Column	Variable	Format	Meaning (units)	Range of Values	Notes
7	1	1	1-10	CRFN	F10.1	Channel radius (F)	> 0.0	If CRFN is input as zero, its value is computed as $1.45\times(1.008665+AW)^{1/3}$. Values given here will be ignored if they also appear in Card Set 4 of the PARameter file (See Table VIB.1). The value for CRFN will be ignored if Card Set 7 is present in the PARameter file.
			11-20	THICK	F10.1	Sample thickness (atoms/barn)		Needed only for TRANSmission or TOTAL cross section or for multiple-scattering corrections
			21-30	DCOVA	F10.1	Constant term in data covariance (default = 0.0)		Data covariance matrix has additional term of the form $(DCOVA + E_i \times DCOVB) \times (DCOVA + E_J \times DCOVB)$. Usually these terms will be set to zero.
			31-40	DCOVB	F10.1	Linear term (default = 0.0)		
			41-50	VMIN	F10.1	Minimum absolute uncertainty (standard deviation) on data	≥ 0	If an experimental uncertainty in your DATa file is smaller than VMIN, SAMMY will increase the value to VMIN.
			51-60	(Currently unused)				
			61-70	DATCR	F10.1	Data at the same energy have correlation DATCR	$-1 \leq$ DATCR ≤ 1	This applies only when a combination of data types are used (see Card Set 8 below).

Table VIA.1 (continued)

Card set	Number of cards	Which card	Column	Variable	Format	Meaning (units)	Range of values	Notes
8	At least 1	1	1-80	CROSS	16A5	Type of data	TRANSmission TOTAL cross section {ELASTic {SCATTering INELAstic scattering DIFFErential elastic {FISSion {REACTion CAPTUre SELF-indication ABSORption ETA	Only those characters in capitals are required (Values connected with curley brackets are equivalent.) Note ABSOR = CAPTU + FISSI Note ETA is defined as NU× (fission/absorption) where NU is specified in Card Set 11 (Card 3) of the PARameter file (Table VIB.1)
							INTEGral	See Sect. V.I page 98s
		2	1-5	NANGLE	I5	Number of angles	> 0	This card is present only for DIFFErential elastic cross sections
			11-20	ANGLE(1)	F10.1	First angle, in laboratory (degrees)	Between 0 and 180°	
			21-30	ANGLE(2)	F10.1	Second angle (degrees)		
			...	...	...	...		
			71-80	ANGLE(7)	F10.1	Seventh angle		
		3,4 etc.	1-10, 11-20, etc.	ANGLE(8) etc.	F10.1	Other angles (degrees)		These cards are absent if NANGLE ≤ 7

Table VIA.1 (continued)

Card set	Number of cards	Which card	Columns	Variable	Format	Meaning (units)	Range of values	Notes
8, cont.	at least 1	5	11-20	DANGLE(1)	F10.1	Angular spread of detector at ANGLE(1) (degrees)		Card is included only for differential elastic cross sections
			21-30	DANGLE(2)	F10.1			
			⋮	⋮	⋮			
			71-80	DANGLE(7)	F10.1			
		6,7,...	1-80	DANGLE(7) to DANGLE (NANGLE)	F10.1	Angular spread		Absent if NANGLE ≤ 7
Alternative to 8	At least 5	1	1-80	CROSS	16A5		COMBInation of TWO types COMBInation of THREE types ⋮ COMBInation of SEVEN types	Columns 16 through 20 indicate how many types of data are to be included, to a maximum of SEVEN
WARNING: This alternative has never been used except for test cases. Contact N. M. Larson when you start to use this option.		2	1-80	$CROSS_1$	16A5	Type of cross section for data set 1		See the other version of Card Set 8
		3	1-10	$EMIN_1$	F10.1	Minimum energy for data set 1 (eV)		These energies override those given in Card Set 2
			11-20	$EMAX_1$	F10.1	Maximum energy for data set 1 (eV)		

Table VIA.1. Continued

Card Set	Number of cards	Which card	Column	Variable	Format	Meaning (units)	Range of Values	Notes
Alt 8, cont.	At least 5	4	1-80	$CROSS_2$	16A5	Type of data for data set 2		
		5	1-10	$EMIN_2$	F10.1	Minimum energy for data set 2 (eV)		
			11-20	$EMAX_2$	F10.1	Maximum energy for data set (eV)		
		etc.	Repeat cards 4 and 5 as many times as necessary, to a maximum of 7 data sets.					
9	1	1	1-10	SPINI	F10.1	Spin of sample nucleus	Integer or half-integer	Positive for even parity and negative for odd; Note that SPINI may be overwritten in Alt Card Set 10
			11-20	ECHAN(1)	F10.1	Excitation energy of the residual nucleus for neutron channel number 1 in an inelastic channel (eV)		Often set to zero. If non-zero, ECHAN is assumed to be defined in the laboratory system for both Coulomb and non-Coulomb channels. Override with alphanumeric commands "CM NON COULOMB EXCITation" or "CM COULOMB EXCITATIon"
			21-25	ISHIFT(1)	I5	Calculate shift for channel 1?	0 = no 1 = yes	
			26-30	LPENT(1)	I5	Calculate penetrabilities for channel 1?	0 = no 1 = yes	If 0, this is a fission channel. If 1, this is a neutron channel. If there is more than one channel, ECHAN(2) is in columns 31-40, ISHIFT(2) in 41-45, LPENT(2) in 46-50, ECHAN(3) in 51-60, etc.

Table VIA.1. Continued

Card Set	Number of cards	Which card	Col-umn	Variable	For-mat	Meaning (Units)	Range of Values	Notes
10	one for each spin group	1	1-10	SPINJ(1)	F10.1			OBSOLETE SPIN GROUP is needed in INPut file to use Card Set 10. In general the author encourages use of the Alternate to Card Set 10 (page 108d)
						(a) spin for resonance in group 1	Integer of half-integer; positive for even parity and negative for odd	Use this option if the sample is pure.
						(b) Spin factor g_J times isotopic abundance, for resonances in group 1	Not integer or half-integer	This option can be used when several isotopes or contaminants are present in the sample; the value which should be inserted here is the product of spin factor and isotopic abundance
			11-15	NENT(1)	I5	Number of particle entrance channels for resonances in group 1	≥ 1, ≤ 3	NENT + NEXT is the total number of particle channels for this spin group. For more than three channels, use Alternate to Card Set 10
			16-20	NEXT(1)	I5	Number of particle exit channels, excluding the entrance channels	≥ 0, ≤ 2	If option (a) for SPINJ is chosen, consistency checks will be made to verify that the various angular moments add up properly. Inconsistencies will result in warning messages, but will not cause SAMMY to abort
			21-25	LSPIN(1,1)	I5	Orbital angular momentum for channel 1 for resonances in group 1	Integer	
			26-30	CHSPIN(1,1)	F5.1	Channel spin for channel 1, group 1	Integer or half-integer	If ENBND>0, then B=$S_l(\alpha)$, where $\alpha = ka$ and k is the center-of-mass momentum for energy ENBND (see Section IIIA.1). If ENBND < 0, then B=ENBND.
			31-40	ENBND(1,1)	F10.1	Boundary condition for channel 1, group 1 (eV)		

Table VIA.1 (continued)

Card set	Number of cards	Which card	Columns	Variable	For-mat	Meaning (Units)	Range of values	Notes
10, cont.	One for each spin group	1, cont.	41-45	LSPIN(2,1)	I5	Orbital angular momen-tum for channel 2 for resonances in group 1	Integer	Card is blank in columns 41-79 if there is only 1 channel (i.e., if NENT=1 and NEXT=0)
			46-50	CHSPIN(2,1)	F5.1	Channel spin for channel 2, group 1		
			51-60	ENBND(2,1)	F10.1	Boundary condition for channel 2, group 1 (eV)		
			61-65	LSPIN(3,1)	I5	Orbital angular momentum for channel 3, group 1		Card is blank in columns 61-79 if there are only 2 channels (i.e., if NENT+NEXT ≤ 2)
			66-70	CHSPIN(3,1)	F5.1			
			71-79	ENBND(3,1)	F9.1			
			80	IXCLD	I1	Flag to exclude this spin group from calculation, but not from PAR or COV files	0 for include 1 for exclude	
		2, etc.						Same as card 1 in this card set, with the quantum numbers appropriate for group number 2

Table VIA.1 (continued)

Card set	Number of cards	Which card	Col-umns	Variable	For-mat	Meaning (Units)	Range of values	Notes
Al-terna-tive to Card Set 10	At least two for each spin group	1	1-3	JJ	I3	Spin group number	1,2,3,...	"USE NEW SPIN GROUP format" must appear in Card Set 3 if this alternative is used. Contact the author if you want more than 999 spin groups
			4	(blank)				
			5	EXCL	A1	Flag if exclude from calculation	blank = include "X" = exclude	
			6-10	NENT(JJ)	I5	Number of entrance channels	> 0	NENT + NEXT is the total number of particle channels for this spin group
			11-15	NEXT(JJ)	I5	Number of exit chan-nels, excluding those which are also entrance channels	≥ 0	
			16-20	SPINJ(JJ)	F5.1	Spin for resonances in group JJ	Integer or half-integer	positive for even parity and negative for odd
			21-30	ABNDNC(JJ)	F10.1	Isotopic abundance for this spin group		
			31-35	SPINI	F5.1	Ground-state spin for this isotope	integer or half-integer	positive for even parity and negative for odd

Table VIA.1 (continued)

Card set	Number of cards	Which card	Col-umns	Variable	For-mat	Meaning (Units)	Range of values	Notes
Alt 10, cont.		2	4-5	N	I2	Channel number	> 0	Note: one card is needed for each channel
			6-8	KZ1(N,JJ)	I3	Charge number Z1 for first particle in this channel	(integer)	
			9-10	LPENT(N,JJ)	I2	Calculate penetra-bility for channel N, spin group J	0 = no 1 = yes	
			11-13	KZ2(N,JJ)	I3	Charge number Z2 for second particle	(integer)	
			15	ISHIFT(N,JJ)	I1	Calculate shift?	0 = no 1 = yes	
			18	IFEXCL(N,JJ)	I1	flag to exclude from final-state calculation	0 = no 1 = yes	
			19-20	LSPIN(N,JJ)	I2	Orbital angular momentum	integer, ≥ 0	
			21-30	CHSPIN(N,JJ)	F10.1	Channel spin	integer or half-integer; sign signifies parity	

Table VIA.1 (continued)

Card set	Number of cards	Which card	Column	Variable	Format	Meaning (units)	Range of values	Notes
Alt. 10, cont.	At least two for each spin group	2, cont.	31-40	ENBND(N,JJ)	F10.1	Boundary condition (eV)		If ENBND>0, then B=$S_l(\alpha)$, where $\alpha = ka$ and k is the center-of-mass momentum for energy ENBND (see Section IIIA.1). If ENBND < 0, then B=ENBND
			41-50	ECHAN(N,JJ)	F10.1	Excitation energy of residual nucleus in an inelastic channel (eV)		See comments for ECHAN in Card Set 9
			51-55	RDEFF(N,JJ)	F5.1	Effective radius (F)	≥ 0	As defined by ENDF; used in calculating phase shift only. If zero, SAMMY uses CRFN from Card Set 7 or PAREFF from Card Set 7 of the PARameter file (Table VIB.1)
			56-60	RDTRU(N,JJ)	F5.1	True radius (F)	≥ 0	As defined by ENDF; used in calculating penetrabilities and phase shifts
			61-70	EMM1(N,JJ)	F10.1	Mass of fragment # 1 (i.e. of target, for channel number 1) (amu)	≥ 0	If zero, uses AW from Card Set 2
			71-80	EMM2(N,JJ)	F10.1	Mass of fragment # 2 (i.e. of neutron, for channel number 1) (amu)	≥ 0	If zero, uses atomic weight of neutron
		3, etc.	Repeat card number 2 for a total of (NENT+NEXT) cards					
		4, etc.	Repeat (Card 1 and Card 2), once for every spin group					
		Last	(blank)					

Table VIA.1 (continued)

Card set	Number of cards	Which card	Column	Variable	Format	Meaning (units)	Range of values	Notes
11	1	1	1-10	THSAMP	F10.1	Sample thickness (cm)	> 0	This card set is present only if self-shielding and multiple-scattering corrections are mentioned in Card Set 3
			11-20	XSAMP	F10.1	Sample height (cm) or sample radius (cm)	≥ 0	
			21-30	YSAMP	F10.1	Sample width (cm) or zero if circular	≥ 0	If XSAMP is given as zero here but XBEAM is positive, the code will set XSAMP = XBEAM, and vice versa. Similarly for YSAMP and YBEAM.
			31-40	XBEAM	F10.1	Beam height (cm) or beam radius (cm), or zero if beam is larger than sample	≥ 0	
			41-50	YBEAM	F10.1	Beam width (cm) or zero if circular or if beam is larger than sample	≥ 0	As of this writing, the rectangular sample is not yet implemented in the code; hence YSAMP and YBEAM are not to be used.
			51-55	NTHETA	I5	Number of points for part of θ-integration	≥ 0 default = 28	
			56-60	NGAUSZ	I5	Number of points for pieces of z-integration	4, 8, or 16 default = 16	
			61-65	NGAUS	I5	Number of points for pieces of integration over cross- section of beam	4, 8, or 16 default = 16	
			66-70	MTHETA	I5	Number of points for rest of θ-integration	≥ 0 default = 11	

Table VIA.1 (continued)

Card set	Number of cards	Which card	Column	Variable	Format	Meaning (units)	Range of values	Notes
12	At least 6	1	1-5	WHAT	A5	Alphanumeric indicator of what comes next	ORRES	Oak Ridge Resolution function (See Sect. IV.E).
		2-11	See Card Set 9 of the PARameter file, Table VIB.1, page 122g, for the remainder of the input for this option. Note that flags to vary the parameters are ignored when values are in the INPut file.					
		12	(blank)					
13	At least 3	1	1-5	WHAT	A5	Alphanumeric indicator of what comes next	RPI R	RPI Resolution function (See Sect. IV.G).
		2-12	See Card Set 14 of the PARameter file, Table VIB.1, page 122s, for the remainder of the input for this option. Note that flags to vary the parameters are ignored when values are in the INPut file.					
		Last	(blank)					
Alter-native to Card Set 13	At least 3	1	1-5	WHAT	A5	Alphanumeric indicator of what comes next	RPI T or RPI C	RPI Resolution function (See Sect. IV.G) with either transmission or capture defaults
		2-12	See Alternative to Card Set 14 of the PARameter file, Table VIB.1, page 122u, for the remainder of the input for this option. Note that flags to vary the parameters are ignored when values are in the INPut file.					
		Last	(blank)					

Table VIA.2 Alphanumeric statements acceptable for use in the INPUT file, Card Set 3

Note: Any of the valid statements listed here may be included in the INPut file, in any order. Usually only the first 20 characters of the statement are required; occasionally other information must be given in specific columns, as indicated below. Characters shown here in lower-case letters are optional in the INPut file, but are included here for clarity. Characters shown here in upper case can be either upper case or lower case in the INPut file, but the cases must not be mixed for any one command. In the event that contradictory statements are included, the last to appear is the instruction that SAMMY will honor. Default instructions need not be included explicitly. Options that are described "for debug purposes" should generally be avoided, because considerable output is generated thereby, especially when many data points are included within the energy range.

Category	Default	Statements	Notes
Input control for experi-mental data	X	DATA ARE IN ORIGINAL multi-style format	Three points per line, relative uncertainties, in 3(2F15.5,F7.3) format. See Section VI.C.1
		DATA FORMAT IS ONE Point per line, *or* USE CSISRS FORMAT For data, *or* CSISRS	The ASCII data file contains one point per line, in (3G11.8) format, with uncertainties being absolute rather than relative
		USE TWENTY SIGNIFICAnt digits, *or* TWENTY	The ASCII data file contains one point per line in (3F20.10) format. Uncertainties are absolute
		DATA ARE IN STANDARd odf format	The data file is the "standard" ODF file with energy in section 1, data in section 2, absolute uncertainty in section 3, and partial derivatives with respect to data-reduction parameters in section 4 ff. See Section V.E.2 of this manual for details
		DATA ARE IN ODF FILE	The data file, whose name you specify either on-line or in your batch file, is in ORELA Data Format. Section 1 contains energies, 2 the data, and 3 the (absolute) uncertainties. See Section VI.C of this report for details
		DIFFERENTIAL DATA ARE in ascii file	See Section VI.C.1 for details
		IMPLICIT DATA COVARIance is wanted	See Section VI.C.2

Table VIA.2 (continued)

Category	Default	Statements	Notes
Input control for experimental data, cont.		ADD CONSTANT TERM TO data covariance	These three statements refer to the option of adding a constant to the data covariance matrix, both on- and off-diagonal, over the energy region in which the effect of the (non-*s*-wave) resonance is felt. Magnitude of this constant is specified in columns 68-80 in the parameter file, for each resonance. For the third option, the default value of this constant is set at 1.E-6 for every non-*s*-wave resonance
	X	DO NOT ADD CONSTANT term to data covariance	
		USE DEFAULT FOR CONStant term to add to data covariance	
		USE TEN PERCENT DATA uncertainty, *or* ADD TEN PERCENT DATA uncertainty	To be used only in nonphysical situations (Second phrase is equivalent to first)
	X	DATA COVARIANCE IS Diagonal	
		DATA HAS OFF-DIAGONAl contribution to covariance matrix of the form $(a + bE_i)(a + bE_j)$	*a* and *b* are specified as DCOVA and DCOVB in the INP file, card set number 7 in Table VIA.1
		DATA COVARIANCE FILE is named YYYYYY.YYY	Substitute your own file name for YYYYYY.YYY in columns 31-40. See Table VIC.2 for the format for this file
Input control for parameters		USE NEW SPIN GROUP Format	See Card Sets 9 and (Alternative to) 10 in Table VIA.1
		USE OBSOLETE SPIN Group format	This option will be removed from future releases of SAMMY; please begin now to use the "new" spin-group format
		INPUT IS ENDF/B FILE 2	Resonance parameters and spin-group quantum number information is taken from an ENDF/B file; see Section VI.G
		USE ENERGY RANGE FROm endf/b file 2	Otherwise, read energy range from INPut file or batch input
		ENERGY UNCERTAINTIES are at end of line in parameter file	See Table VIB.1, Card Set 1, columns 68-80, second alternative

Table VIA.2 (continued)

Category	Default	Statements	Notes
Input control for parameters, cont.		IGNORE INPUT BINARY covariance file, *or* IGNORE	Your PARameter file specifies that the parameter covariance matrix is kept in a binary file. For this particular run, however, you wish to pretend that there were no previous runs generating such a file; instead you wish to use the large (ideally ∞) uncertainties that indicate no prior knowledge of parameter values
	X	LAB NON COULOMB EXCItation energies	The excitation energy (for channels for which there is no Coulomb interaction) is defined in the laboratory rather than the center of mass system. See parameter ECHAN in Card Set 9 or Card Set 10 of the INPut file, Table VIA.1
		CM NON COULOMB EXCITation energies	The non-Coulomb excitation energies are given in the com system rather than the laboratory system
	X	LAB COULOMB EXCITATIon energies	For Coulomb channels, the excitation energy or Q-value ECHAN (Card Set 9 or 10 of the INPut file) is in the laboratory system
		CM COULOMB EXCITATIOn energies	For Coulomb channels, the excitation energy or Q-value ECHAN (Card Set 9 or 10 of the INPut file) is in the center of mass system
Line-printer control options	X	DO NOT PRINT ANY INPut parameters	
		PRINT ALL INPUT PARAmeters	
		PRINT VARIED INPUT Parameters	Resonances for which no parameters are flagged will not be printed. Use this option for direct comparison with output parameters, which are always printed in this mode
	X	DO NOT PRINT INPUT Data	Note that this refers to experimental values of the measured cross section (or transmission, etc.), as read in from the DATa file (see Section VI.C)
		PRINT INPUT DATA	
	X	DO NOT PRINT THEORETical values	Often these are available in the ODF file (see Table VIIC.1) so they need not be printed in the LPT file
		PRINT THEORETICAL VAlues	
	X	DO NOT PRINT PARTIAL derivatives	
		PRINT PARTIAL DERIVAtives	Use this option only for debug purposes

Table VIA.2 (continued)

Category	Default	Statements	Notes
Line-printer control options, cont.	X	DO NOT SUPPRESS INTErmediate printout	Updated parameter values and covariance matrix elements are printed after completion of each energy region
		SUPPRESS INTERMEDIATe printout	Updated parameter values and covariance matrix elements are printed only upon completion of entire run
		DO NOT SUPPRESS ANY intermediate printout	Updated parameter values are printed after each iteration of Bayes' equations (i.e., typically twice for each energy region). Updated covariance matrix elements are evaluated and printed only upon completion of an energy region
	X	DO NOT USE SHORT FORmat for output	
		USE SHORT FORMAT FOR output	Resonance parameters are printed in the LPT file (Section VII.A), in F12.4 format rather than E format. Even though this may produce more legible output, often fewer significant digits will be printed
	X	DO NOT PRINT REDUCED widths	
		PRINT REDUCED WIDTHS	Reduced width amplitudes will be printed in the LPT file (Section VII.A), along with the square root of the resonance energies. That is, what are printed are the "u-parameters" as described in Section III of this report
		DO NOT PRINT SMALL Correlation coefficients	Any line of the correlation matrix whose off-diagonal elements are small will not be printed. "Small" is defined less than ICORR/100 in abslute value, where ICORR is specified in Card Set 2 (Table VIA.1)
	X	DO NOT PRINT DEBUG Information	
		PRINT DEBUG INFORMATion, *or* DEBUG	Use for debug purposes only on short runs
		PRINT CAPTURE AREA in lpt file	The capture area, defined as $A = g\Gamma_n\Gamma_\gamma/\Gamma$, is printed in the SAMMY.LPT file

Table VIA.2 (continued)

Category	Default	Statements	Notes
Constants	X	USE ENDF VALUES For constants, *or* USE 1999 ENDF-102 Constant values	SAMMY is now using those values for the physical constants which have been "blessed" by ENDF (See Appendix E)
		USE 1995 ENDF-102 Constant values, *or* USE OLDER VALUES OF constants	
		USE SAMMY-K1 DEFAULts for constants	This will give the values which "USE PRECISE VALUES Of constants" used to give
Operation control for standard runs	X	SOLVE BAYES EQUATIONs	Update parameter values and covariances via Bayes' equations
		DO NOT SOLVE BAYES Equation	Parameter values are not updated, but remain fixed. Theoretical values of transmission or cross section are evaluated for each energy region specified, using these fixed parameter values
	X	REICH-MOORE FORMALISm is wanted, *or* MORE ACCURATE REICH-moore, *or* XCT	See Section III.D. Note that "more accurate" refers to the computational method, not to the formalism
		ORIGINAL REICH-MOORE formalism, *or* CRO	See Section III.A. This method of calculating the RM formalism is sometimes inaccurate, particularly at low energies for capture
		MULTILEVEL BREIT-WIGner is wanted, *or* MLBW FORMALISM IS WAnted, *or* MLBW	See Section III.C
		SINGLE LEVEL BREIT-WIgner is wanted, *or* SLBW FORMALISM IS WAnted, *or* SLBW	See Section III.C
	X	LET SAMMY CHOOSE WHIch inversion scheme to use	
		USE (N+V) INVERSION scheme	Original method; Section II.B.1.a
		USE (I+Q) INVERSION scheme	See Section II.B.1.b

Table VIA.2 (continued)

Category	Default	Statements	Notes
Operation control for standard runs, cont.		USE POLAR COORDINATEs for fission widths	When there are two channels for fission, the pair may be treated as a vector, in which case the two independent variables are the magnitude of the vector and the polar angle, rather than the two widths. Compare, for example, with the Vogt formalism [EV58]
	X	DO NOT DIVIDE DATA Into regions - do entire energy range at once	
		DIVIDE DATA INTO REGions with a fixed number of data points per region	SAMMY will automatically choose energy regions of NEPNTS (see Card Set 2, Table VIA.1) data points each, for sequential analysis. Warning: SAMMY merely counts; it does not consider carefully whether dividing point is located in a region where the theoretical values (σ or T) are nonlinear with respect to the parameters. Dividing in such a location (at or near a resonance) will invalidate the linearity assumption used in deriving Bayes' equation, and thus lead to spurious results. Users are urged to use this option only on the "zeroth pass," as an aid in deciding where to divide the data, and not for final runs
	X	DO NOT USE S-WAVE CUtoff	
		USE S-WAVE CUTOFF	Non-*s*-wave resonances far away from the data being analyzed are omitted in parts of the calculation of the R-matrix. The definition of "far away" used in setting the partial derivatives to zero is $\lvert E - E_\lambda \rvert > 20 \left(\sum_c \Gamma_{\lambda c} + \Gamma_\lambda^\gamma \right) + 3(d + r)$, where d and r are Doppler and resolution widths, respectively. The definition of "far away" for the contribution to the imaginary part of R is 100 times that for the derivatives; contributions to the real part of R are always included For *s*-wave resonances, the user may choose whether to use a similar cutoff. If a cutoff is desired, its value is twice that for non *s*-wave resonance Caution: Though SAMMY will run faster with the cutoff option invoked, results may not be as accurate

Table VIA.2 (continued)

Category	Default	Statements	Notes
Operation control for standard runs, cont.		MODIFY UNVARIED WIDths when varying radii	This option is no longer available in versions M5 (2000) and higher
	X	DO NOT MODIFY UNVARied widths when varying radii	The partial widths are assumed to be constant when varying the channel radius; hence the reduced width amplitudes may vary. In version M2 of the code, derivatives with respect to the channel radius were not properly calculated for this option. In versions M5 and higher, derivatives are properly calculated; this is the only option available for those versions of the code.
		CHI SQUARED IS NOT Wanted, *or* DO NOT PRINT LS CHI squared	Remember that in Bayes' (as opposed to least-squares) χ^2 is an irrelevant quantity and is therefore not even calculated. Nevertheless it is often useful for comparing results of different fits. For each energy region, χ^2 may be calculated from $\chi^2_{LS} = \sum_i (D_i - T_i)\,(V^{-1})_i\,(D_i - T_i)$
	X	CHI SQUARED IS WANTEd, *or* PRINT LS CHI SQUARED	is calculated, and χ^2 and χ^2/ NDAT (where NDAT is the number of data points in that region) are reported. Note that SAMMY does not report χ^2/ dof (where dof = degrees of freedom = NDAT-NPAR, with NPAR being the number of parameters), since with Bayes' method dof can be zero or negative.
	X	DO NOT PRINT BAYES Chi squared unless it can be easily generated without additional calculations	In addition to χ^2, the quantity we choose to call the Bayesian χ^2 may also be reported, where $\chi^2_B = \sum_{i,j} (D_i - T_i)\,(N+V)^{-1}_{ij}\,(D_j - T_j)$ Caveat: Theoretical values T_i are generated using the values of the parameters prior to analysis of this energy region

Table VIA.2 (continued)

Category	Default	Statements	Notes
Operation control for standard runs, cont.	X	DO NOT PRINT WEIGHTEd residuals; *or* DO NOT PRINT LS WEIGhted residuals	Two types of weighted residuals may be printed. The least-squares weighted residual is defined as $R_{ii}^{LS} = \sqrt{(V^{-1})_{ii}}\,(D_i - T_i)$,
		PRINT WEIGHTED RESIDuals; *or* PRINT LS WEIGHTED Residuals	where D is the experimental data, V its covariance matrix, and T the theoretical value evaluated at the initial values of the parameters. The Bayesian weighted residual is defined as
	X	PRINT BAYES WEIGHTED residuals	$R_i^B = \sum_j (N+V)_{ij}^{-1}\,(D_j - T_j)$, where $N_{kn} = \sum_{ij} \frac{\partial T_k}{\partial u_i} M_{ij} \frac{\partial T_n}{\partial u_j}$ and M_{ij} is the initial covariance matrix element for parameters u_i and u_i
		DO NOT PRINT BAYES Weighted residuals	
	X	DO NOT PRINT PHASE shifts	In the LPT file
		PRINT PHASE SHIFTS For input parameters	
Broadening options	X	BROADENING IS WANTED	Some form of broadening is to be used; see Section IV
		BROADENING IS NOT WAnted	If you do not wish to have SAMMY Doppler- or resolution-broaden the theoretical values, be sure to remove Card Sets 5 and 6 (see Table VIA.1) from the INP file, as well as include this card
	X	USE FREE GAS MODEL Of doppler broadening, *or* FGM	The free-gas model of Doppler broadening, as described in Section IV.F, is to be used
		USE LEAL,HWANG DOPPLer broadening	The Doppler-broadening method of Leal and Hwang, as described in Section IV.D, is to be used
		USE MULTI-STYLE DOPPPler broadening, *or* HEGA	High-energy Gaussian approximation to the free-gas model is to be used for Doppler broadening, as described in Section IV.A.1

Table VIA.2 (continued)

Category	Default	Statements	Notes
Broadening options, cont.		NO LOW-ENERGY BROADENing is to be used	Theoretical values are not to be broadened below the energy value ELOWBR given in Card Set 5 of Table VIA.1 (the INPut file). This option works only with the original (MULTI-style) broadening, and not with the Leal-Hwang method nor with the free-gas model
		USE TRUE TOTAL CROSS section for resolution broadening	Usually total cross sections will be converted to transmissions after Doppler broadening, before resolution broadening. This command forces the use of the total cross section rather than the transmission for resolution broadening. See test case tr81 for an example
		EXPONENTIAL FOLDING width is energy-dependent	See Section IV.A.2.b, Eq. (IVA2b.6)
		DO NOT SHIFT ENERGY for exponential tail on resolution broadening	See Section IV.A.2.c; the energy shift ΔE_s is assumed zero here
	X	SHIFT ENERGY FOR EXPonential tail on resolution broadening	See Section IV.A.2.c; the energy shift ΔE_s is chosen to give a maximum of the integrand at the resonance energy
Multiple-scattering corrections	X	USE SELF SHIELDING Only, no scattering, *or* SELF SHIELD	Only self-shielding is to be included; no single- or double-scattering (see Section III.F)
		USE SINGLE SCATTERINg plus self shielding, *or* SINGLE	Include self-shielding plus single-scattering corrections
		INCLUDE DOUBLE SCATTering corrections, *or* DOUBLE, *or* USE MULTIPLE SCATTERing plus single scattering	Include self-shielding, single-scattering, and double-scattering corrections (See Section III.F)
		INFINITE SLAB	Single-scattering correction does not include edge-effects
	X	FINITE SLAB	Edge effects corrections are included
	X	MAKE NEW FILE WITH Edge effects	See Section III.F. This statement is ignored if "INFINITE SLAB" is specified.
		FILE WITH EDGE EFFECts already exists	

Table VIA.2 (continued)

Category	Default	Statements	Notes
Multiple-scattering corrections, cont.		MAKE PLOT FILE OF Multiple scattering pieces	Store Y0, Y1, and Y2 in file SAM53.DAT, to be read by program SAMCMP
		NORMALIZE AS CROSS Section rather than yield, *or* CROSS SECTION	See Section III.F
	X	NORMALIZE AS YIELD Rather than cross section, *or* YIELD	
		NORMALIZE AS (1-E)SIgma	
Angular distribution data		USE LABORATORY CROSs sections	For differential elastic scattering; see Section III.E
	X	USE CENTER-OF-MASS cross sections	
		OMIT FINITE SIZE CORrections	
		INCIDENT NEUTRON ATTenuation is included	
		APPROXIMATE SCATTERED neutron attenuation is wanted, *or* SCATTERED NEUTRON ATtenuation is included	These two are equivalent statements
Special options		ENDF/B-VI FILE 2 IS wanted, *or* ENDF	Resonance parameters are to be provided in the format required for ENDF/B-VI File 2 (Reich-Moore representation) is wanted. See Section VI.F for details
		RECONSTRUCT CROSS Section from resonance parameters	SAMMY will automatically choose an appropriate grid and evaluate total, elastic, capture, and fission cross sections on that grid, using NJOY method. See Section V.G
		ARTIFICIAL ENERGY grid is needed	SAMMY will automatically choose an appropriate grid and evaluate, using SAMMY method. See Section V.G
	X	DO NOT AVERAGE OVER energy ranges	
		AVERAGE OVER ENERGY ranges	Produce energy-averaged experimental data and theoretical values, using output parameters from an earlier SAMMY analysis. See Section V.C.1 for details

Table VIA.2 (continued)

Category	Default	Statements	Notes
Special options, cont.		GROUP AVERAGE OVER Energy ranges; *or* BONDARENKO AVERAGE Over energy ranges	Produce Bondarenko-weighted averages, using output parameters from an earlier SAMMY analysis. See Section V.C.2 for details
		MAKE NO CORRECTIONS to theoretical values	Do not perform Doppler or resolution broadening corrections, nor include normalizations or backgrounds, before averaging
		MAXWELLIAN AVERAGED capture cross sections are wanted, *or* STELLAR AVERAGED Capture cross sections are wanted	Generate stellar averaged capture cross section; see Section V.F
		CALCULATE MAXWELLIAN averages after reconstructing cross sections	
		ADD CROSS SECTIONs from endf/b file 3	For use in generating Maxwellian averages; see Table VID.5 and VIH.1
	X	DO NOT PERFORM SUMMARy analysis	
		PERFORM SUMMARY ANALysis	Evaluate and print the summed strength function and the corresponding covariance matrix. Note: SAMMY stops upon completion of this task
		GENERATE PARTIAL DERivatives only	SAMMY will assume all resonance parameters, and only resonance parameters, are to be varied; that Bayes' equations are not to be solved; and that the partial derivatives of the theory with respect to those parameters is to be output in file SAMMY.PDS
		GENERATE SPIN GROUP cross sections	Generate ODF (Plot) file containing energy (from auxiliary grid) in Section 1, unbroadened cross section in Section 2, spin-group-1 contribution to unbroadened cross section in Section 3, spin-group-2 contribution in Section 4, etc.
		REFORMULATE DATA FOR implicit data covariances	See Sections II.A.1.a and VI.C.3
		UNRESOLVED RESONANCE region, *or* FRITZ FROEHNERS FITAcs, *or* FITACS	Use the SAMMY version of Fritz Froehner's code FITACS for analysis of the unresolved resonance region

Table VIA.2 (continued)

Category	Default	Statements	Notes
Special options, cont.		COMPARE EXPERIMENT To theory	See Section VIII.K; results are reported in binary file SAM53.DAT
		GENERATE Y AND W MATrices, *or* YW READ Y AND W MATRICES, *or* WY	See Section II.B.3 for a description of the M+W form of Bayes' Equations. See Test Case tr89 for examples of the use of this option.
		STOP *abc n*	Cease execution prior to the *n*th occurrence of segment *abc* (note that there are two spaces before *n* in this command). Used only for debug (Section XI.B page 211) and preparation for Monte Carlo calculations (Section VIII.O page 150z.7)
Plot file control	X	DO NOT GENERATE PLOT file automatically	The output ODF file is described fully elsewhere (Table VIIC.1). To complete all sections of this file requires (1) initialization; (2) running SAMMY without solving Bayes' equations to obtain theoretical values determined by the input parameters; (3) solving Bayes' equations to obtain updated parameter values; and (4) obtaining theoretical values determined by the updated parameters. That is, the ODF file requires an initialization plus three complete passes through SAMMY. The option to GENERATE ODF (or PLOT) FILE AUtomatically does all this busy-work for you. If you do not need plots, do not use this option. Note to users who do not have ODF plotting package: SAMMY is now able to produce a binary file containing the information that would normally be included in the ODF file. It is strongly recommended that users without the ODF option extract the information from this binary file rather than from the LPT file. A FORTRAN file mbin.f is available as a guide for reading the binary file (whose name is also SAMMY.ODF); comment cards in the FORTRAN file explain how to link SAMMY to produce the binary rather than the ODF file
		GENERATE ODF FILE AUtomatically; *or* GENERATE PLOT FILE Automatically	

Table VIA.2 (continued)

Category	Default	Statements	Notes
Plot file control, cont.		ODF FILE IS WANTED-- XXXXXX.XXX, ZEROth order guess ODF FILE IS WANTED-- XXXXXX.XXX, FINAl guess	These statements are all ignored if you choose to GENERATE ODF FILE automatically. To use these options, replace XXXXXX.XXX (columns 21-30) with the name of your ODF file. Be sure that file already contains energies and data (Sections 1,2,3, and possibly 6 and 7; see Table VIIC.1)
		PLOT UNBROADENED Cross sections	Generate file SAMMY.UNB which contains the auxiliary energy grid in Section 1 and the unbroadened theoretical values in Sections 2 etc. SAMMY also generates an ASCII file samunb.dat with the same information in CSISRS format
	X	DO NOT INCLUDE THEORetical uncertainties in plot file INCLUDE THEORETICAL uncertainties in plot file	The covariance matrix element connecting theory point T_i with point T_j is $$\sum_{k,n} \frac{\partial T_i}{\partial u_k} M_{kn} \frac{\partial T_j}{\partial u_n} \quad ,$$ where M_{kn} is the covariance matrix element connecting parameter u_k with parameter u_n. The theoretical uncertainty on theory T_i is the square root of the diagonal element; that is, $$\Delta T_i^2 = \sum_{k,n} \frac{\partial T_i}{\partial u_k} M_{kn} \frac{\partial T_i}{\partial u_n}$$ The values ΔT_i are reported in Sections 10 and 11 (or 6 & 7) of the ODF file
		PLOT RESOLUTION FUNCtion	See Section VIII.L

Table VIB.1 (continued)

Card set, No. of cards	Which card	Column	Variable name	Format	Meaning (units)	Values	Notes
6, at least 4	1	first few	WHAT	A5	Alphanumeric indicator of what comes next	NORMAlization and background	Only the first five characters are required
	2,4, etc	1-10	ANORM	F	a = normalization (dimensionless)	generally ~ 1.0	See Section V.E.1 for a complete description of normalization and background parameters
		11-20	BACKA	F	B_a = constant background (dimensionless if data is transmission, barns if cross section)		
		21-30	BACKB	F	B_b = background proportional to $1/\sqrt{E}$ or linear in time ($\sqrt{\text{eV}}$ or barns$\times\sqrt{\text{eV}}$)		When the data are angular distributions, Card 2 contains normalization and backgrounds for the first angle, Card 4 for the second, etc.
		31-40	BACKC	F	B_c = background proportional to $\sqrt{E}$ or linear in inverse time ($1/\sqrt{\text{eV}}$ or barns$/\sqrt{\text{eV}}$)		
		41-50	BACKD	F	B_d = coefficient for exponential background (dimensionless or barns)		
		51-60	BACKF	F	B_f = exponential decay constant ($\sqrt{\text{eV}}$)		
		61-62	IF(1)	I2	Vary ANORM?	-1 or 0 for no 1 for yes	A negative value here indicates that the value of this parameter is changed from earlier runs; only unvaried parameters may be changed in this fashion
		63-64	IF(2)	I2	Vary BACKA?		
		65-66	IF(3)	I2	Vary BACKB?		
		67-68	IF(4)	I2	Vary BACKC?		
		69-70	IF(5)	I2	Vary BACKD?		
		71-72	IF(6)	I2	Vary BACKF?		
	3,5, etc.	1-10	DNORM	F	Absolute uncertainty on ANORM		
		11-20	DBACKA	F	Absolute uncertainty on BACKA		
		21-30	DBACKB	F	Absolute uncertainty on BACKB		
		31-40	DBACKC	F	Absolute uncertainty on BACKC		
		41-50	DBACKD	F	Absolute uncertainty on BACKD		
		51-60	DBACKF	F	Absolute uncertainty on BACKF		
	Last	(blank)					

Table VIB.1 (continued)

Card set, No. of cards	Which card	Column	Variable name	For-mat	Meaning (units)	Values	Notes
7, at least 3	1	First few	WHAT	A5	Alphanumeric indicator of what comes next	RADIUs parameters come next	Only the first five characters are required
	2	1-10	PAREFF	F10	Radius (F) to be used for potential scattering	> 0.0	
		11-20	PARTRU	F10	Radius (F) to be used for penetrabilities and shifts, or (if negative), Negative of the ratio of the mass of the sample nucleus to that of a neutron	(a) Greater than zero	Use value given
						(b) Negative	The (absolute value) of the number given is the ratio of mass of the sample nucleus to that of a neutron. SAMMY then calculates PARTRU using 1.23 $(AWRI)^{1/3}$ + 0.8 which is the ENDF formula, converted to FERMI
						(c) 0.0	SAMMY uses the value of CRFN from INPut file or from Card Set 4 of PARameter file for PARTRU
		21	ICHAN	I1	Channel flag	0 if applies to every channel 1 if applies to certain specified channels only	
		22	IFLEFF	I1	Flag to indicate whether PAREFF is to be varied	0 if not varied > 0 if varied	

Table VIB.1 (continued)

Card Set, No. of cards	Which card	Col-umn	Variable name	For-mat	Meaning (units)	Values	Notes
11 cont., at least 3	4	1-5	WHAT	A5	Descriptor for this card	FINIT	Finite-size corrections for differential elastic cross sections
		7	IFLAGI	I1	Flag to indicate whether parameter ATTNI is to be varied	0 or 1	
		9	IFLAGO	I1	Flag to indicate whether parameter ATTNO is to be varied	0 or 1	
		11-20	ATTNI	F10	Incident-neutron attenuation (atoms/barn)		See Section III.E
		21-30	DTTNI	F10	Uncertainty on ATTNI (atoms/barn)		This card may be omitted if not needed. This card may be repeated, once for each angle. If the card occurs only once, the same attenuations are used for each angle
		31-40	ATTNO	F10	Scattered-neutron attenuation (atoms/barn)		
		41-50	DTTNO	F10	uncertainty on ATTNO (atoms/barn)		
	5	1-5	WHAT	A5		GAMMA	Use the same radiation width for all resonances in this spin group. Γ_γ is assumed to be varied.
		6-7	IG	I2	Spin group number		
		11-20	GAMGAM	F10	Reduced radiation width for all resonances in spin group IG		
		21-30	DGAM	F10	Uncertainty on GAMGAM		This card may be omitted
	6	1-5	WHAT	A5		TZERO	See Section III.A.2.c for description
		7	IFTZER	I1	Flag whether to vary t_0	0 or 1	
		9	IFLZER	I1	Flag whether to vary L_0	0 or 1	
		11-20	TZERO	F10	t_0 (μs)	0.0	
		21-30	DTZERO	F10	Uncertainty on t_0 (μs)		
		31-40	LZERO	F10	L_0 (dimensionless)	1.0	
		41-50	DLZERO	F10	Uncertainty on L_0 (dimensionless)		
		51-60	DIST	F10	Flight path length (m)		This value for fpl is used only if DIST is zero (see INPut File, Card Set 5, page 104)

Table VIB.1 (continued)

Card Set, No. of cards	Which card	Col-umn	Variable name	For-mat	Meaning (units)	Values	Notes
11, cont.	7	1-5	WHAT	A5		SIABN	Abundances for self-indication transmission sample
		6-7	IF1	I2	Flag to vary SIABND(1)		
		8-9	IF2	I2	Flag to vary SIABND(2)		
		10	IF3	I1	Flag to vary SIABND(3)		Note that nuclides are defined
		11-20	SIABN(1)	F10	Abundance for nuclide # 1		in Card Set 10, which must
		21-30	dSIABN(1)	F10	Uncertainty for nuclide # 1		occur before Card Set 11 in
		31-40	SIABN(2)	F10	Abundance for nuclide # 2		the PARameter file
		41-50	dSIABN(2)	F10	Uncertainty for nuclide # 2		
		51-60	SIABN(3)	F10	Abundance for nuclide # 3		Repeat this card until all
		61-70	dSIABN(3)	F10	Uncertainty for nuclide # 3		nuclides have been included
	8	1-5	WHAT	A5		SELFI	Temperature and thickness for
		6-7	IFTEMP	I2	Flag to vary temperature	0 or 1	transmission sample for self
		8-9	IFTHCK	I2	Flag to vary thickness	0 or 1	indication experiment
		11-20	SITEM	F10	Effective temperature for self-indication transmission sample		
		21-30	dSITEM	F10	Uncertainty on tempreature SITEM		This card may be omitted
		31-40	SITHC	F10	Thickness (atoms/barn)		
		41-50	dSITHC	F10	Uncertainty on thickness SITHC		

Table VIB.1 (continued)

Card Set, No. of cards	Which card	Column	Variable name	For-mat	Meaning (units)	Values	Notes
11 cont., at least 3	9	1-5	WHAT	A5		EFFIC	Efficiency for capture and for fission for eta calculation
		6-7	IFCAPE	I2	Flag to vary capture efficiency	0 or 1	
		8-9	IFFISE	I2	Flag to vary fission efficiency	0 or 1	
		11-20	EFCAP	F10	Efficiency for detecting capture events		
		21-30	EFFIS	F10	Efficiency for detecting fission events		
		31-40	dEFCAP	F10	Uncertainty on capture efficiency		
		41-50	dEFFIS	F10	Uncertainty on fission efficiency		This card may be omitted
	10	1-5	WHAT	A5		DELTE	Delta-E is energy-dependent as described
		7	IFLAG1	I2	Flag to vary DELE1	0 or 1	on page 69, Section IV.A.2.b, Eq.
		9	IFLAG0	I2	Flag to vary DELE0	0 or 1	(IVA2b.7)
		10	IFLAGL	I1	Flag to vary DELE2	0 or 1	
		11-20	DELE1	F10	Coefficient of E in Eq. (IVA2b.7) (m / eV)		
		21-30	D1	F10	Uncertainty on DELE1		
		31-40	DELE0	F10	Constant term in Eq. (IVA2b.7) (m)		
		41-50	D0	F10	Uncertainty on DELE0		
		51-60	DELE2	F10	Coefficient of log term in Eq. (IVA2b.7) (m / ln(eV))		
		61-70	D2	F10	Uncertainty on DELE2		This card may be omitted if unneeded
	Last	(blank)					

Table VIB.1 (continued)

Card Set, No.	Which card	Column	Variable name	Format	Meaning (units)	Values	Notes
12, at least 4	1	1-5	WHAT	A5	Alphanumeric indicator of what comes next	PARAMagnetic	Paramagnetic cross section parameters are given here (see Section V.H)
	2	1-5	WHAT	A5	Which particular nuclide	TM , ER , HO	(Two letters followed by three blanks)
		6-7	IFA	I2	Flag whether to vary *A*		
		8-9	IFB	I2	Flag whether to vary *B*		
		10	IFP	I1	Flag whether to vary *P*		
		11-20	*A*	F	*A* of Eq. (VH.1)		See Section V.H for default values
		21-30	*dA*	F	Uncertainty on *A*		
		31-40	*B*	F	*B* of Eq. (VH.1)		
		41-50	*dB*	F	Uncertainty on *B*		
		51-60	*P*	F	*P* of Eq. (VH.1)		
		61-70	*dP*	F	Uncertainty on *P*		
	3	6-7	ISO	I2	Isotope (nuclide) number for this paramagnetic cross section	1	
		8-9	IFC	I2	Flag whether to vary *C*		
		11-20	*C*	F	*C* of Eq. (VH.1)		
		21-30	*dC*	F	Uncertainty on *C*		
	Last	(blank)					

Table VIB.1 (continued)

Card Set, No. of cards	Which card	Column	Variable name	Format	Meaning (units)	Values	Notes
14, at least 3	1	first few	WHAT	A5	Alphanumeric indicator of what comes next	RPI Resolution function	First five characters must be present; the rest are optional
	2	1-5	WHAT	A5	Descriptor for this card	BURST	Burst width is on this card
		6	*ip*	I1	Flag whether to vary burst width	0 or 1	
		11-20	*p*	F10	Full width at half max of burst (ns)		See Table IVG.1 on page 92v for default values
		21-30	d*p*	F10	Uncertainty on burst width		
	3	1-5	WHAT	A5	Descriptor for this card	TAU (two spaces needed)	This card gives parameters for τ from Eq. (IVG1.5)
		6-10	$i\tau 1$,$i\tau 2$, $i\tau 3$,$i\tau 4$ $i\tau 5$	5I1	Flags whether to vary τ_i for $i = 1$ to 5	0 or 1 for each	
		11-20	TAU1	F10	τ_1 from Eq. (IVG1.4) pg 92u		See Table IVG.1, page 92v
		21-30	TAU2	F10	τ_2		
		31-40	TAU3	F10	τ_3		
		41-50	TAU4	F10	τ_4		
		51-60	TAU5	F10	τ_5		
		61-70	TAU6	F10	τ_6		
		71-80	TAU7	F10	τ_7		
	4	6	$i\tau 6$	I1	Flag whether to vary τ_6	0 or 1	
		7	$i\tau 7$	I1	Flag whether to vary τ_7	0 or 1	
		11-80	DTAUi	5F10	Uncertainties on τ_i		

Table VIB.1 (continued)

Card Set, No. of cards	Which card	Col-umn	Variable name	Format	Meaning (units)	Values	Notes
14, cont.	5	1-5	WHAT	A5	Descriptor for this card	LAMBDa	
		6	ILAM0	I1	Flag whether to vary Λ_0	0 or 1	
		7	ILAM1	I1	Flag whether to vary Λ_1	0 or 1	
		8	ILAM2	I1	Flag whether to vary Λ_2	0 or 1	
		9	ILAM3	I1	Flag whether to vary Λ_3	0 or 1	
		10	ILAM4	I1	Flag whether to vary Λ_4	0 or 1	
		11-20	LAM0	F10	Value of Λ_0		
		21-30	LAM1	F10	Value of Λ_1	See Eq. (IVG1.3) and Table IVG.1	
		31-40	LAM2	F10	Value of Λ_2		
		41-50	LAM3	F10	Value of Λ_3		
		51-60	LAM4	F10	Value of Λ_4		
	6	11-60	DLAM0	F10	Uncertainty on LAM0		
			DLAM1	F10	Uncertainty on LAM1		
			DLAM2	F10	Uncertainty on LAM2		
			DLAM3	F10	Uncertainty on LAM3		
			DLAM4	F10	Uncertainty on LAM4		

Table VIB.1 (continued)

Card Set, No. of cards	Which card	Column	Variable name	Format	Meaning (units)	Values	Notes
14, cont.	7	1-5	WHAT	A5	Descriptor for this card	A1 (That's "A one, 3 blanks")	
		6	IAA1	I1	Flag whether to vary a_1	0 or 1	
		7	IAA2	I1	Flag whether to vary a_2	0 or 1	
		8	IAA3	I1	Flag whether to vary a_3	0 or 1	
		9	IAA4	I1	Flag whether to vary a_4	0 or 1	
		10	IAA5	I1	Flag whether to vary a_5	0 or 1	
		11-20	AA1	F10	a_1		
		21-30	AA2	F10	a_2	See Eq. (IVG1.5) and Table IVG.1	
		31-40	AA3	F10	a_3		
		41-50	AA4	F10	a_4		
		51-60	AA5	F10	a_5		
		61-70	AA6	F10	a_6		
		71-80	AA7	F19	a_7		
	8	6	IAA6	I1	Flag whether to vary a_6	0 or 1	
		7	IAA7	I1	Flag whether to vary a_7	0 or 1	
		11-80	DAAi	7F10	Uncertainties on a_1		

Table VIB.1 (continued)

Card Set, No. of cards	Which card	Col-umn	Variable name	Format	Meaning (units)	Values	Notes
	9	1-5	WHAT	A5	Descriptor for this card	EXPON	
		6	IT0	I1	Flag whether to vary t_0	0 or 1	
		7	IA2	I1	Flag whether to vary A_2	0 or 1	
		8	IA3	I1	Flag whether to vary A_3	0 or 1	
		9	IA4	I1	Flag whether to vary A_4	0 or 1	
		10	IA5	I1	Flag whether to vary A_5	0 or 1	
		11-20	T0	F10	t_0		
		21-30	A2	F10	A_2	See Eq. (IVG1.2) and Table IVG.1	
		31-40	A3	F10	A_3		
		41-50	A4	F10	A_4		
		51-60	A5	F10	A_5		
	10	11-60	DT0, DAi	5F10	Uncertainties on t_0 and A_i		
	11	1-5	WHAT	A5	Descriptor for this card	CHANNel crunch boundaries	
		7	ICH	I1	Flag whether to vary channel width	0 or 1	
		11-20	ECRNCH	F10	Highest energy for this channel width c (eV)		
		21-30	CH	F10	Value for channel width c (nsec)	See Section IV.G.1	
		31-40	DCH	F10	Uncertainty on channel width (nsec)		
	12, etc.	Just like 11			Repeat card 11 as many times as needed, end with blank card		
	Last	(blank)					

Table VIB.1 (continued)

Card Set, No. of cards	Which card	Col-umn	Variable name	For-mat	Meaning (units)	Values	Notes
Alterna-tive to 14, at least 1	1	first few	WHAT	A5	Alphanumeric indicator of what comes next	RPI Transmission resolution function *or* RPI Capture resolution function	First five characters (capitalized) must be present; the rest are optional
	2-10	Default values for transmission or capture, as defined in Table IVG.1 on page 92 w, will be used. No input is needed here.					
	11	1-5	WHAT	A5	Descriptor for this card	CHANNel crunch boundaries	
		7	ICH	I1	Flag whether to vary channel width	0 or 1	
		11-20	ECRNCH	F10	Highest energy for this channel width *c* (eV)		
		21-30	CH	F10	Value for channel width *c* (nsec)	See Section IV.G.1	
		31-40	DCH	F10	Uncertainty on channel width (nsec)		
	12, etc.	Just like 11			Repeat card 11 as many times as needed, end with blank card		
	Last	(blank)					

Table VIB.1 (continued)

Card Set, No. of cards	Which card	Col-umn	Variable name	For-mat	Meaning (units)	Values	Notes
15, at least 3	1	first few	WHAT	A5	Alphanumeric indicator of what comes next	DETECtor efficiencies	First five characters must be present; the rest are optional
	2	1-10	PARDET(1)	F10	Detector efficiency appropriate for these spin groups	≥ 0	See Section V.K page 98u.
		11-20	DELDET(1)	F10	Uncertainty on this detector efficiency		
		21-22	IFLDET(1)	I2	Flag whether to vary this detector efficiency	0 = do not vary 1 = vary	
		23-24	IGRDET(1,1)	I2	Number of the first spin group belonging to this isotope		If more than 29 spin groups are needed, insert "-1" in Columns 79-80, and continue on the next line with (16I5) format. When there are more than 99 spin groups altogether, all I formats on Card 2 are changed from I2 to I5
		25-26	IGRDET(2,1)	I2			
		etc.					
	3, etc.	repeat card 2 for second (third, etc.) detector efficiency					
	Last	(blank)					

VI.C THE DATa and Data CoVariance FILES

Several possible formats are offered for inputting experimental data into the current version of SAMMY; these are described in Subsection VI.C.1. ASCII versions include the original (MULTI-style) data file with three data points per line, a format consistent with CSISRS data, and a twenty-significant-digit format to meet the need for high precision.

Two distinct treatments of data covariance matrices are provided. The first, which is denoted the "explicit" covariance, is provided directly by the user and is described in Section VI.C.2. The second is denoted the "implicit" data covariance (idc) because the covariance matrix is never generated per se; rather, the matrices necessary for the proper solution of Bayes' equations (see Section II.A.1) are generated from input provided by the user. The idc option is described in Section VI.C.3.

VI.C.2. Explicit Data Covariance Matrices

Two options for off-diagonal data covariance matrices are available within SAMMY. The first, which is labeled "explicit," is treated as a regular off-diagonal covariance matrix; see the description of Bayes' Equations, Section II. Use of the explicit data covariance matrix thus requires inversion of an $N \times N$ array, where N is the number of data points. The second, "implicit" data covariance matrix (described in Section II.A.2) is input as a specific mathematical form, and is treated by a more sophisticated mathematical process that does not require inversion of such a large matrix. When either formulation could be used, the implicit is recommended since the implementation is more efficient.

Table VIC2.1 shows the format for a data covariance (DCV) file, to be included when each covariance matrix element is given explicitly. The name of this file must be specified in Card Set 3 of the INPut file (Tables VIA.1 and VIA.2) in columns 31-40 of the Card reading "DATA COVARIANCE FILE is named . . ."

Occasionally it may be convenient to introduce a constant on- and off-diagonal data covariance in the neighborhood of a non-*s*-wave resonance, permitting effective decoupling of any underlying $l = 0$ state from the non-*s* waves. This is effective because an additive constant covariance is mathematically equivalent to a constant, coherent correction term for either the

Table VIC2.1 Format of the Data CoVariance file

Card	Column	Variable	Format	Meaning
1	1-10	VARDAT(1,1)	F10.1	Variance for data point 1
2	1-10	VARDAT(2,1)	F10.1	Covariance between data points 1 and 2
	11-20	VARDAT(2,2)	F10.1	Variance for data point 2
3	1-10	VARDAT(3,1)	F10.1	Covariance between data points 1 and 3
	11-20	VARDAT(3,2)	F10.1	Covariance between data points 2 and 3
	21-30	VARDAT(3,3)	F10.1	Variance for data point 3
4	1-10 ...	VARDAT(4,1) etc.	F10.1	

Note that the ordering of data points is **low** to **high** (independent of the ordering in the DATa file), and only those data points actually used in the calculation can be referenced in the DCV file. A maximum of eight matrix elements are to be included on one line; thus "card number 11", for example, will actually be two lines, with eight numbers on the first and three on the second.

data or the theory. (Algebraic details are presented in Appendix A of the original SAMMY report [NL80].) This type of off-diagonal data covariance matrix can be generated automatically by SAMMY; details for input are given in Table VIA.2 under the category "Input Control" and in Card Set 1, columns 68 to 80, of Table VIB.1.

Another type of explicit off-diagonal data covariance matrix which can be automatically generated by SAMMY is of the form

$$V^{ij} = \bar{V}^{ij} + (a+bE^i)(a+bE^j) \quad , \qquad \text{(VIC2.1)}$$

where $\bar{V}^{ij}$ is provided by the user, E^i is the energy for data point i, and a and b are constants chosen by the user. This type of covariance is useful if there are energy-dependent coherent uncertainties in the data, for example, if a subtracted background is imperfectly known. Input for this option is given in Card Set 7 of Table VIA.1, and the "Input Control" statement "DATA HAS OFF-DIAGONAL contribution . . ." of Table VIA.2.

VI.C.3 Implicit Data Covariance Matrices

As described in Section II (*Bayes' Equations*) it is possible for SAMMY to treat certain types of data covariances without actually generating the complete off-diagonal data covariance matrix. These types are labeled Implicit Data Covariances (IDC) and may be understood as follows:

The data-reduction process, which is generally performed by the experimentalist who measured the data, includes background subtraction and normalization, as well as other corrections (for deadtime, self-shielding, etc.). This process produces off-diagonal data covariance matrix (i.e., systematic errors), which should then be included (along with statistical errors) in the analysis process. To reconstruct the covariance matrix due to the background and normalization corrections, SAMMY assumes that the "corrected" data D and the "original" data R are related via

$$D(E) = \frac{R(E) - b(E)}{a} \quad , \qquad \text{(VIC3.1)}$$

in which a and b are defined as in Section V.E.1 (*Explicit Normalization and/or Background Functions*). Corrections applied to the experimental data are opposite to those applied to the theory; that is, for experimental data the background is subtracted before dividing by normalization, and theoretical values are first multiplied by the normalization before adding the background.

Values and uncertainties (as well as possible correlations) for the normalization and parameters should be determined by the experimentalist. However, the analyst may wish to apply further corrections to the data. In this case, the analyst can run SAMMY, including normalization and/or background functions in the parameter file with the parameters flagged (varied) in order to determine the correct values for the parameters. The next step would be to produce a modified data file; this step can be accomplished with SAMMY by including a command line "REFORMULATE DATA FOR implicit data covariance" in the INPut file. SAMMY will then produce a file SAMMY.DA2 in the same format as the analyst's DATa file, with the data values corrected according to Eq. (VIC2.2). Note that uncertainties in this data file will not be changed (except to divide by the normalization a, if the uncertainties in the file are absolute rather than relative): This file, like the original, contains only statistical, but not systematic, errors. SAMMY will also produce a file SAMMY.IDC which contains the normalization & broadening information, and a new parameter file SAMMY.PA2 identical to the analyst's PAR file except for the absence of the normalization and broadening information. The uncertainties in SAMMY.IDC can then be modified (or added) to be the proper experimental uncertainties on the normalization and broadening parameters, to be used in further SAMMY runs.

In subsequent SAMMY runs for that data set, the INPut file contains the command line "IMPLICIT DATA COVARIance matrix is to be used." SAMMY then looks for the IDC file, which uses the same formats as portions of the PARameter file. In particular, Card Set 6

(NORMAlization and background) and Card Set 13 (BACKGround functions) can be included in this file; see Section V.E.1 on page 98g for a description of these functions. Any correlations between values should also be given here, using again the formats of the PARameter file for EXPLIcit uncertainties (Card Set Last, first alternative).

Within SAMMY, the Implicit Data Covariance information is treated as described in Section II.A.1.a, page 14a. Note that the SAMMY user need never generate off-diagonal data covariances directly.

For examples on the use of IDC, see test case TR70.

VI.E. THE AVeraGe FILE

In Sect. V.C (page 98a and following), descriptions are given of the way SAMMY can be used to produce energy- averaged, time-averaged, or Bondarenko-averaged cross sections and the associated covariance matrix. To invoke these options, alphanumeric command cards must be included in the INPut file. For energy- or time-averaging (Section V.C.1, page 98b.1), the command is

```
AVERAGE OVER ENERGY ranges.
```

For Bondarenko averaging, the command is

```
GROUP AVERAGE OVER Energy ranges, or
BONDARENKO AVERAGE Over energy ranges.
```

One or more additional files are required, which are denoted the AVG (AVeraGe) files or BON (BONdarenko) files; their names are given to SAMMY on unit 5 (teletype or batch; see Table VID.4), directly following the first data file. Formats for AVG files are given in Table VIE.1, and for the BON files in Table VIE.2. Note that the two types of files follow very much the same format, except the BON files require additional input parameter values.

Table VIE.1. Format of the AVG file

Card Number	Col-umn	Variable Name	Format	Meaning (units)	Possible Values	Notes
1	1-80	TITLE	A80			
2	1-10	TYPE	A10	type of averaging to be used	"energy-ave" or "time-avera"	energy- or time- average
3	1-10	EMIN	F10.x	Minimum energy for this range (eV)		
	11-20	EMAX	F10.x	Maximum energy for this range (eV)		If EMAX = 0, use EMAX = EMIN from next card
4, 5, ...	(repeat Card 3 as many times as needed)					
last	(blank)					

Table VIE.2. Format of the BONdarenko file

Card Number	Col-umn	Variable Name	Form at	Meaning (units)	Possible Values	Notes
1	1-80	TITLE	A80			
2	1-10	TYPE	A10	type of averaging to be used	"bondarenko" in either upper or lower case	Currently this is the only option; others may be added later
3	1-10	EMIN	F10.x	Minimum energy for this range (eV)		
	11-20	EMAX	F10.x	Maximum energy for this range (eV)		If EMAX = 0, use EMAX = EMIN from next card
4,5,...	(repeat Card 3 as many times as needed)					
6	(blank)					
7	1-10	TYPE	A10	type of parameters to be used	"bondarenko" in either upper or lower case	Again this is the only option; others may be added later
8	1-10	ebonda(1)	F10.x	Energy (eV)		
	11-20	bondar(1)	F10.x	Value of $C(E)$ at E = ebonda(1)		Eq. (VC2.2)
	21-30	sig000	F10.x	σ_0		Eq. (VC2.2)
9	1-10	ebonda(2)	F10.x	Energy (eV)		
	11-20	bondar(2)	F10.x	Value of $C(E)$ at E = ebonda(2)		
10, 11,...	(Repeat Card 9 as many times as needed. Value of $C(E)$ is interpolated linearly between the points specified.)					
last	(blank)					

VI.F TO PRODUCE A FILE IN ENDF-6 FORMAT

SAMMY is capable of converting information obtained from the usual SAMMY INPut and PARameter files (plus a modest amount of additional input) into ENDF-6 File 2 format, using what ENDF-102 calls the "Reich-Moore representation." To invoke this option you need to include the following card in your INPut file:

ENDF/B-VI FILE 2 IS WANTED

(This may be shortened to "ENDF" if desired.) In addition, you will create a new file, whose name you supply to SAMMY in the site in which SAMMY would normally expect the DATa file name. Contents of this file are shown in Table VIF.1. SAMMY will produce a file called SAMMY.NDF, which contains the appropriate cards for ENDF-6 File 2.

In SAMMY.NDF, resonance energies are given in F format, to as many significant digits as possible given the limitation of eleven columns. Widths are given in E format, with, however, the "E" suppressed and the exponent given as one digit if possible. The angular momentum parameter AJ is specified as $\pm J$, where the sign denotes the channel spin s (AJ = $-J$ denotes $s = I - i$, with $i = 1/2$ for neutron; AJ = $+J$ denotes $s = I + i$.); this is in compliance with the format change approved by the Cross Section Evaluation Working Group at the November, 1999, meeting [ENDF 99].

Table VIF.1 ENDF Input File

Card Set	Card Number	Variable	For-mat	Notes
1	1	ZA AWR	F F	These are ENDF variables, and thus follow the ENDF-6 rules for determining their values. Often, but not always, ZA has the value (1000 * Z + A). AWR is the ratio of the mass of the sample to the neutron mass (ratio-to-neutron is standard ENDF units).
		LRF	I	LRF specifies which ENDF format is to be used; LRF = 3 (Reich-Moore) is default.
		MAT	I	ENDF MAT number (default = 99).

Card Set	Card Number	Variable	For-mat	Notes
2	1	SPI(1) ZAI(1) ABN(1) AWRI(1)	F	These are also ENDF-6 variables, and are defined respectively as the ground state spin, the (Z,A) value, the abundance, and the ratio of the isotopic mass to that of a neutron. The default for AWRI(i) is AW/*aneutron*, where AW is the value given in the SAMMY files and *aneutron* is the mass of a neutron.
	2	LENDFG(1,1)	I	Angular momentum for the first ENDF spin group
		KENDFG(1,1,1) KENDFG(2,1,1) . . .	I I	SAMMY spin groups that belong to this ENDF spin group. Note that there may be more than one SAMMY group per ENDF group, since ENDF groups consist of energy-ordered sets of all resonances with the same L, while SAMMY groups are defined by both J and L. SAMMY will check to be sure the groups you specify have the correct L-value, and give you an error message if they don't.
	3	LENDFG(i,1)	I	Angular momentum for ith group (2nd, 3rd, etc.)
		KENDFG(1,i,1) KENDFG(2,i,1) . . .	I I	SAMMY groups belonging to this ENDF group
	4	Repeat Card 3 as many times as necessary		
	Last	(blank)		
3	Repeat Card Set 2 as many times as necessary, once for each nuclide			

VI.G USING ENDF/B FILE 2 AS INPUT TO SAMMY

Instead of manually creating a SAMMY-type PARameter file and an entire SAMMY-type INPut file, a user may retrieve resonance parameters (File 2) from the Evaluated Nuclear Data Files (ENDF) Library [NNDC] and use that file directly as input to SAMMY. The first portion of a SAMMY-type INPut file is still required; this file contains Card Sets 1-8 but no others (see Table VIA.1). Included in Card Set 3 of the INPut file must be the line

```
INPUT IS ENDF/B FILE
```

The name of the ENDF/B File-2 file is included in the input stream where the name of the PARameter file is called for.

Output from a run using an ENDF file for input includes two additional files not usually found in SAMMY output. The first is SAMNDF.INP which is a SAMMY-type INPut file containing the spin group information in Card Sets 9 and 10. The second is a SAMMY-type PARameter file containing the resonance parameter information from the ENDF file, translated into SAMMY formats. These two files can then be used for subsequent SAMMY runs.

Caveat: Only isotopic ENDF files can be used in this fashion. For example, one could use the file for ^{28}Si but not the file for natural silicon. Note also that it is *only the File-2 portion of the ENDF file* which is to be included; that is, the user must extract File 2 from the complete ENDF file before using it as input to SAMMY. SAMMY has no provisions for reading and/or using other portions of the ENDF file. [The one exception is in the evaluation of the stellar averages, for which ENDF File 3 may be included. See Section VI.H for details.]

VI.H FORMAT OF THE MXW FILE

In order to generate stellar (Maxwellian) averages of capture cross sections (see Section V.F), two pieces of input are needed. In the alphanumeric portion (Card Set 3) of the INPut file, the line

```
MAXWELLIAN AVERAGED capture cross sections are wanted
```

or

```
STELLAR AVERAGED CAPture cross sections are wanted
```

must be included (the two phrases are treated identically within the code). It is also necessary to specify the temperatures at which the stellar averages are to be calculated; these are given in a "MXW" file whose name is specified immediately following the name of the DATa file in the input stream. The format of the MXW file is one temperature per line, in F10.1 format, in units of eV.

When calculating stellar averages, it is often desirable to include cross sections at energies above the resolved-resonance region. In SAMMY, this may be done by providing the "smooth cross section" in the ENDF File 3 format. Users must also include the following line

```
ADD CROSS SECTIONs from endf/b file 3
```

in the alphanumeric portion of the INPut file.

For users unfamiliar with ENDF formats, a description of the relevant portions of File 3 is presented in Table VI.H.1. Note that the parameter INT specifies an interpolation scheme for NBL energy points. For INT = 1, the cross section from E_i to E_{i+1} is constant and equal to C_i. For INT = 2, the cross section for $E_i < E < E_{i+1}$ is linearly interpolated between the two values. [Note that other options are available in ENDF but only these two have been implemented in SAMMY.]

Examples for stellar averaging are given in Test Cases tr42, tr49, and tr51.

Table VIH.1. Format for File-3 cross sections to be added for stellar averages

Card Number	Variable	Col-umns	Format	Notes
1	(Nothing on this card is important to SAMMY runs)			
2	NR	45-55	I11	Number of energy regions
	NP	56-66	I11	Total number of energy points to be specified
3	NBT(1)	1-11	I11	Number of energy points in region 1
	INT(1)	12-22	I11	Interpolation type for region 1 (INT=1 implies constant, INT=2 implies linear; contact the SAMMY author if other options are needed.)
	NBT(2)	23-33	I11	Number of energy points in region 2
	INT(2)	34-44	I11	Interpolation type for region 2
	NBT(3)	45-55	I11	Number of energy points in region 3
	INT(3)	56-66	I11	Interpolation type for region 3
4,5, ...	Repeat Card 3 until all NR regions have been specified. Note that the sum of the NBT values must equal NP.			
6	E(1)	1-11	F11.x	First energy value
	C(1)	12-22	F11.x	Value of cross section at energy E(1)
	E(2)	23-33	F11.x	Next energy value
	C(2)	23-44	F11.x	Value of cross section at energy E(2)
	E(3)	45-55	F11.x	Next energy value
	C(4)	56-66	F11.x	Value of cross section at energy E(3)
7,8,...	Repeat Card 6 until all NP energy points have been specified			

VII.A LINE-PRINTER OUTPUT

The first two output files (the "LPT" and the "IO" files) are intended for visual inspection. The LPT file contains full output, detailed to the extent specified by the user in the INPut file (see Table VIA.1 and .2).

The IO file merely lists initial and final parameter values; at some point in the near future, the author intends to eliminate the IO file unless there is great demand to maintain it.

The LPT file contains a wealth of information with which users should become familiar. Here you find, among other things,

- Input file names;
- Title for the run (taken from your INPut file);
- Values for varied and fixed parameters;
- Verbatim alphanumeric commands (with notification if the command is not recognized);
- Chronological listing of the SAMMY segments used in the run;
- Updated parameter values, uncertainties, and correlation values;
- Chi-squared values;
- Error messages, if applicable.

Sample LPT files may be found among the output for the test cases or for the tutorial exercises. See Sections XI.D and X.D respectively.

It is strongly recommended that novice SAMMY users examine the LPT file for each run, to be sure SAMMY is interpreting input as the user intended. Even experienced SAMMY users should regularly look at the LPT file, especially when output parameter values or chi-squared values are puzzling or when the run ends abnormally. Such problems are often the result of user input errors, which can frequently be discovered by comparing intended input values with the values as listed in the LPT file. In addition, the LPT file often provides error messages to guide the user into fixing an input error. Error messages are also provided for abnormal aborts for common input errors. (Please notify the author if you have suggestions for a more informative error message for your favorite mistake.)

VII.B OUTPUT TO BE USED AS INPUT

The next two output files (the "PAR" and the "COV" files) are intended to be used as input to another SAMMY run. The PAR file is as described in Sect. VI.B, with the "third alternative" chosen for the "last" Card Set of Table VIB.1.

In very early versions of SAMMY, the output "binary COVariance file" contained only the new (updated) covariance matrix for physical parameters (i.e., **not** for the u-parameters; see Sect. II.C). Output parameter values were stored in the output PARameter file. When these two files were used as input to another run, the covariance matrix for the u-parameters was generated from Eq. (IIC.1).

Two drawbacks to this scheme led to expansion of the COV file. First, unnecessary computer time was spent in making the conversion back to u-parameters. Second, and more important, was the loss of precision between runs. In converting from u- to physical parameters, storing these in ASCII format, reading them back in for the next run, and converting back to u-parameters, often the last several significant digits were lost. One would expect that analysis of two energy regions, first in two separate executions of SAMMY, then in one execution but still analyzing the two regions sequentially, should give identical results. With the early storage scheme, small differences occurred; with the current scheme, no discrepancies are found.

In the current storage scheme, the output PARameter file has not changed from earlier versions. However, SAMMY users should be aware that

If a COVariance file is specified, SAMMY will use parameter values given in the (binary) COVariance file rather than those given in the PARameter file.

That is, all parameter values are taken from the values stored in the binary COVariance file; these values are more precise than those in the PARameter file. The few exceptions to this rule occur only for certain unvaried (and properly flagged) parameters; see Table VIB.1 for specifics.

Table VIIB.1 shows which variables are written in what order in the COVariance file. Dotted lines separate values kept in separate records.

Occasionally a user may wish to modify the contents of the COVariance file (and associated PARameter file), in order to de-activate a measurement-related parameter (e.g., sample thickness or Doppler temperature) and activate the comparable parameter for the measurement to be analyzed next. This may be accomplished using the program SAMAMR; see Sect. VIII.A for details.

Table VIIB.1 Binary COVariance file

Variable names (with dimension in parenthesis)	Meaning
Title	test which version of the SAMMY code wrote this COV file
JJJJJJ(200)	array dimensions, etc.
ALLVR(NPAR)	covariance matrix for physical parameters, stored in NPAR separate records
VRPR(NPAR)	covariance matrix for u-parameters, stored in NPAR separate records
U(NPAR)	values of u-parameters
PKEN(NRES)	resonance energies
GGA(NRES)	gamma widths
GSI(NTOTC,NRES)	particle widths
IFLRES(NTOTC2,NRES)	ordinal numbers for varied resonance parameters
IGROUP(NRES)	number of the spin group to which the resonance belongs
BETAPR(NTOTC,NRES)	(related to particle widths)
GBETPR(3,NRES)	(related to gamma widths)
BETA(NTRIAG,NRES)	(related to particle widths)
POLAR(2,NRES)	optional; fission width in polar coordinant system
IFLPOL(2,NRES)	optional; ordinal numbers for varied polar fission widths
IFLEXT(NREXT,NTOTC,NGROUP)	ordinal numbers for varied R-external parameters
PAREXT(NREXT,NTOTC,NGROUP)	R-external parameters

Variable names (with dimension in parenthesis)	Meaning
IGRRAD(NGROUP), PAREFF(NUMRAD), IFLEFF(NUMRAD), PARTRU(NUMRAD), IFLTRU(NUMRAD)	values of the several radii, spin groups to which they apply, and ordinal numbers for varied radii
AMUISO(NUMISO), PARISO(NUMISO), IFLISO(NUMISO), IGRISO(NGROUP)	weight, fractional abundance, parameter numbers, spin groups which correspond to this isotope
PARDET(NUMDET)	detector efficiency parameters for eta measurements
IFLDET(NUMDET)	ordinal numbers for detector efficiencies
IGRDET(NUMDET)	
PARBRD(NUMBRD)	"broadening" parameters
IFLBRD(NUMBRD)	ordinal numbers for varied broadening parameters
DUM(19)	related to broadening parameters
PARMSC(NUMMSC)	values of miscellaneous parameters
NAMMSC(NUMMSC)	names of miscellaneous parameters
IFLMSC(NUMMSC)	ordinal numbers for miscellaneous parameters
PARPMC(NUMPMC)	values of "unused" parameters
IFLPMC(NUMPMC)	ordinal numbers for paramagnetic parameters
ISOPMC(NUMPMC)	
PARORR(NUMORR)	parameters related to the Oak Ridge Resolution function option
IFLORR(NUMORR)	
ECRNCH(NUMORR-11)	
ENDETS(NMDETS)	
SESESE(NMDETS)	
ESESES(NMDETS)	
SIGDTS(NMDETS)	

Variable names (with dimension in parenthesis)	Meaning
PARRPI(NUMRPI), IFLRPI(NUMRPI), ECRNCH(NUMRPI-NNNRPI)	parameters related to the RPI Resolution function option
PARBGF(NUMBGF), IFLBGF(NUMBGF), KNDBGF(NUMBGF), BGFMIN(NUMBGF), BGFMAX(NUMBGF)	parameters related to the background function option
PARDTP(NUMDTP)	values of data reduction parameters
NAMDTP(NUMDTP)	names of data reduction parameters
IFLDTP(NUMDTP)	ordinal numbers for varied data reduction parameters
PARUSD(NUMUSD)	values of "unused" parameters
NAMUSD(NUMUSD)	names of unused parameters
IFLUSD(NUMUSD)	ordinal numbers for unused parameters
PARBAG(NUMBAG)	values of "baggage" parameters
NAMBAG(NUMBAG)	names of baggage parameters
IFLBAG(NUMBAG)	ordinal numbers for baggage parameters

VIII. AUXILIARY PROGRAMS

A number of "auxiliary" programs, not an integral part of SAMMY itself, are designed to be used in conjunction with SAMMY. These programs manipulate SAMMY PARameter and/or COVariance files, aid in interpreting or illustrating SAMMY input or output, or offer a means of comparing SAMMY results with other calculations.

In Section VIII.A the program SAMAMR is described; this program is used to rearrange PARameter and COVariance files to facilitate analyses of disparate data sets with the same resonance parameter set. (Note that SAMAMR replaces the two codes SAMADD and SAMMIX described in earlier versions of this report.)

The program SAMEST is described in Section VIII.B; SAMEST will estimate the storage requirements for SAMMY, based on information provided interactively by the user; this information includes such items as the number of resonances, how many parameters are varied, and how many data points are to be included. (Note: with the advent of modern computing facilities, use of this program is not as crucial as in the past. Hence little time has been spent maintaining this program. It is the author's intention to render this program completely irrelevant in the near future, by converting the code to FORTRAN 90.)

Program SAMORT, described in Section VIII.C, is used for plotting the components of the Oak Ridge resolution function. Similar plots can be made for the RPI resolution function using program SAMRPT (Section VIII.M) and of the original MULTI-style resolution function (Section VIII.L).

The program SAMCNV, described in Section VIII.D, was designed to read a SAMMY binary COVariance file and produce an ASCII file containing the complete covariance matrix for all resonance parameters.

The program SAMSTA, described in Section VIII.E, is used to create a file from which "staircase plots" of the resonance from a SAMMY PARameter file can be generated.

Program SAMPLT, which provides an alternative methodology for generating plots, is discussed in Section VIII.F. (Note: This program has been renamed from SAMBIN.)

Section VIII.G describes program SAMTHN, a simple program for averaging data files used as input to SAMMY runs.

When angular distribution data are analyzed, results are reported in an ODF file [JC78] from which plots can be made of energy vs cross section at a fixed angle. To plot angle vs cross section at fixed energy, it is necessary to reorganize the ODF file; this reorganization is accomplished with program ANGODF, discussed in Section VIII.H.

Quantum numbers can be generated using program SAMQUA, described in Section VIII.I.

The task of converting from REFIT to SAMMY input can be eased by use of program CONVRT, discussed in Section VIII.J.

For assistance in comparing results of calculations performed by different computer codes, use program SAMCMP; see Section VIII.K for details.

Program LEVDEN is described in a separate manual [NL89, not yet completed]. LEVDEN is used to fit the level-density formula of Gilbert and Cameron to the number of levels (as given in a SAMMY PARameter file) in a specified energy region.

Program SAMDIS (elsewhere named SAMDIST) is used for calculating statistical distributions for R-Matrix resonance parameters; see ref. [LL95]. Level spacing distributions are calculated according to the Wigner distribution law, distributions for widths are calculated via χ^2 distributions, and long-range correlations of the energies are tested via the Δ_3 statistic of Mehta-Dyson. A summary of features of this code is given in Section VIII.N, along with recent modifications of the input to the code.

Program SAMSMC may be used for Monte-Carlo calculations of the self-shielding and multiple-scattering corrections to capture and fission yields. See Section VIII.O.

VIII.A SAMAMR: ADD, MIX, OR RECOVER VARIABLES

Because the fitting procedure in SAMMY is Bayes' method (Section II) rather than ordinary least-squares, SAMMY may be used for general evaluation purposes: that is, for determining a set of parameters which simultaneously describe a large number of different types of experimental data taken at different times and/or at different laboratories. Numerous examples of such evaluations are given in the references of Appendix D, "Analyses Using SAMMY."

Performing such evaluations with SAMMY presently requires sequential analyses of the various data sets,[1] with the output parameter and covariance matrix from the first analyses used as input to the second, output from the second used as input to the third, etc. If none of the broadening parameters are varied during the analyses, and if no data-reduction parameters are included, this will pose no undue difficulty; the analyst simply changes the values of the thickness and/or of the broadening parameters in the INPut file to correspond to the data currently being analyzed. However, when any of the broadening parameters are varied, and/or when normalization or background are included in the analysis, the PARameter and COVariance files must also correspond to the current data set. The code SAMAMR performs the appropriate modifications to the PARameter and COVariance files.

For example, data may come from two or more samples of different thicknesses and at different temperatures. The initial PARameter file is set up to include thickness and temperature appropriate for the first sample; thickness and temperature for the other samples are simply omitted. After the analysis of the first data set, code SAMAMR is used to incorporate the second thickness (as yet uncorrelated to any other parameters) and to "mothball" the correlated but now-to-be-unused first thickness; a second run of SAMAMR introduces the new temperature parameter and mothballs the old. The resulting PARameter file can then be used as input for the SAMMY analysis of the second data set. If, for a subsequent SAMMY run, one of the "UNUSED" parameters must be resurrected, SAMAMR will interchange the current BROADening parameter with the appropriate UNUSED parameter.

To illustrate, suppose three data sets are available, taken from three samples at two different temperatures:

Data Set 1: Sample 1 (thickness n_1, Temperature T_1)
Data Set 2: Sample 2 (thickness n_2, Temperature T_2)
Data Set 3: Sample 3 (thickness n_3, Temperature T_1)

The sequence of commands required to properly analyze these data is shown in Table VIIIA.1. The input PARameter file (TR7AAA.PAR) is listed in Table VIIIA.2. Output PARameter files are listed in Tables VIIIA.3 through VIIIA.12. (Data and analysis are courtesy

---

[1] A planned reformulation of the implementation of Bayes' method within SAMMY will provide an alternative to this procedure. See Appendix F for details.

of F. G. Perey [FP84].) Note that values (and covariances) of the unused parameters are updated in each SAMMY run, even though the data have no direct effect on those parameters. Rather, the effect is indirect, via the covariance matrix. Note also that values are never changed in a SAMAMR run. Complete listings of all INPut, PARameter, DATA, and LPT files for this example are given in test case TR7, which is available along with the SAMMY FORTRAN from the Radiation Safety Information Computational Center [RSICC].

SAMAMR was designed to be run interactively (though it can be run in batch once the user is sufficiently familiar with the input). The code will prompt the user with questions about the type of operation to be performed, the parameters involved, and values for any new parameters.

Type of operation. The first question asked by SAMAMR is "Do you want to Add, Mix, Remove, reCover, or Introduce variables?"; the user will type the capitalized letter for the appropriate operation.

The operations Add and Mix correspond respectively to the operations performed by the old codes SAMADD and SAMMIX. Add refers to (1) the removal of one parameter to the unused list and (2) the introduction of another parameter (of the same kind) into the active list. The user is asked to specify the particular parameter (from a list provided), to give the variable number for that parameter if it was varied in the run which produced this covariance file, and to give the value and uncertainty to be used for the new parameter. Mix refers to the interchange of one unused parameter with the corresponding parameter in the active variable set. The user must provide the location (variable number) within the unused parameter set.

The operations Remove, reCover, and Introduce are used to reorganize the attenuation or normalization-and-background parameters when the analysis involves both angle-differential data (such as the elastic angular distribution scattering data) and other data which are integrated over angle (such as transmission). The operation Remove moves normalization-and-background parameters for all angles, or attenuation parameters for all angles, from the active variable set to the unused variable set. The operation reCover performs the inverse, moving parameters from the unused to the active set. Introduce allows the introduction of new parameter values and uncertainties when switching from analysis of angle-integrated data to analysis of angular distribution data.

Type of parameter. The types of parameters to be treated by SAMAMR are different, depending on the operation to be performed.

For both Add and Mix, only one parameter is treated at a time; the example shown in Table VIIIA.1 therefore requires two runs of SAMAMR between each run of SAMMY. The parameters that can be treated are taken from the following list, in which is also given the Card Set and Card number from the PARameter file (see Table VIB.1):

(Broadening parameters)

TEMP , THICK, DEL-L, DEL-G, DEL-E	(Card Set 4, Card 3)

(Normalization and background parameters)

NORML, BACKA, BACKB, BACKC, BACKD, BACKF	(Card Set 6, Card 2)

(ORR resolution parameters)

BURST	(Card Set 9, Card 2)
WATR0, WATR1, WATR2	(Card Set 9, Card 3)
TANTA	(Card Set 9, Card 3)
X1, X2, X3, X0	(Card Set 9, Card 4)
WWW, ALPHA	(Card Set 9, Card 6)
D, F, G	(Card Set 9, Card 8)
DELTA	(Card Set 9, Card 8)
CHANN	(Card Set 9, Card 10)

(Miscellaneous parameters, with alternative names in square brackets)

DELTA, DELT2 [DELL1, DELL0]	(Card Set 11, Card 2)
NU [ETA]	(Card Set 11, Card 3)
ATTNI, ATTNO [FINIT, FINI2]	(Card Set 11, Card 4)
TZERO, LZERO	(Card Set 11, Card 6)
SIABN	(Card Set 11, Card 7)
SITEM, SITHC [SELFI]	(Card Set 11, Card 8)
EFFIC, FISEF [EFCAP, EFFIS]	(Card Set 11, Card 9)
DELTE, DELE0, DELE2 [DELE1, DELE0, DELE2]	(Card Set 11, Card 10)
CONCR, CONTR	(Card Set 11, Card 11)

(RPI resolution function parameters)

BURST	(Card Set 14, Card 2)
TAU	(Card Set 14, Card 3)
LAMBD	(Card Set 14, Card 5)
A1	(Card Set 14, Card 7)
EXPON	(Card Set 14, Card 9)
CHANN	(Card Set 14, Card 11)

In addition to giving the parameter name, as given in the above list, the user will sometimes also need to specify which parameter of this type is to be used. The name is given in the first five columns (be sure to leave blanks if the name is fewer than five characters), and an integer number is then given. For the RPI resolution parameters, the second, third, etc., variable on the Card (in the PARameter file) are specified by "2", "3", etc. in the SAMAMR input. See test case tr87 for examples of this.

For the operations Remove, reCover, and Introduce, only the parameters ATTEN and ALLNB may be specified. When ATTEN is specified, all attenuation parameters (both incident and outgoing, from Card Set 11, Card 4 of the PARameter file) are involved. When ALLNB is specified, all normalization and background parameters are involved (see Card Set 6, Card 2). Again, only one type can be be treated during one run of SAMAMR.

When the operation Introduce is used, attenuation or normalization/background parameters are assumed to be given in a separate file in the same format as used in the PARameter file (though without the "MISCEllaneous parameters" or "NORMAlization and background" header lines of Card Sets 11 and 6). SAMMY will ask for the file name instead of the parameter values. Test case tr36 shows examples of the use of this feature.

An additional restriction for operations Remove, reCover, and Introduce stems from the connection between the attenuation parameters and the number of angles: SAMAMR assumes that removal of attenuation parameters implies changing from angular-distribution data to angle-integrated data, and that recovery or introduction of attenuation parameters implies the reverse change. Removal of attenuation parameters, therefore, must be accomplished *after* removal of normalization and background parameters, and recovery or introduction of attenuation parameters must be accomplished *prior to* recovery or introduction of normalization and background parameters.

Test cases tr7, tr32, tr36, tr79, and tr87 all have examples of the use of program SAMAMR.

VIII.B SAMEST: ESTIMATE ARRAY SIZES

Array sizes in SAMMY are allocated dynamically during the execution of the program (see Sect. XI.A for details); this permits more efficient use of the computer's capacity, allowing larger amounts of data to be analyzed within one SAMMY run. Because arrays do not have fixed dimensions, it is not possible to give an absolute maximum number of resonances, number of varied parameters, or number of data points that can be included in any one run; those maximum numbers are interdependent and not easily specified in general. The program SAMEST was therefore developed to provide an estimate of the amount of storage required for the particular configuration of parameters and data that the user has in mind. SAMEST can be used to decide whether a data set should be analyzed in two (or more) pieces, or whether the values of some parameters should be held fixed. SAMEST is designed to run interactively, so that the user can test as many configurations as needed within one SAMEST run. SAMEST will give the estimate of the array size (in number of single precision words) needed for each segment of SAMMY, based on answers to its questions. Questions posed by SAMEST are listed in Table VIIIB.1 and an example (for an early 1988 ORELA VAX/VMS version of SAMMY) shown in Table VIIIB.2.

With the advent of modern high-speed and large-memory computers, the importance of the capability to estimate array sizes has declined considerably. Hence this auxiliary program has not been well-maintained in recent years. With release of version M5 of the SAMMY code, program SAMEST is still available but will not provide accurate estimates. With subsequent releases of the code, this program is likely to be eliminated completely.

Table VIIIB.1. Questions asked by SAMEST.

QUESTIONS	ANSWERS
HOW MANY GROUPS?	The number of spin groups as defined in the INPut file
HOW MANY RESONANCES?	the number of resonances in the PARameter file
HOW MANY PARTICLE CHANNELS ALTOGETHER?	the total number of channels; the maximum of the sum of NENT(i) and NEXT(i) from Card Set 10 in the INPut file
Do you wish to give complete input?	Y or N; if answer is not Y, questions beginning with an asterisk are omitted.
*IS R-EXT INCLUDED?	Y or N (Sect. III.A.1.a)
*ARE NORMALIZATION AND/OR BACKGROUND INCLUDED?	Y or N (Sect. V.E.1)
*HOW MANY "DATA" PARAMETERS?	number of data reduction parameters (Sect. V.E.2)
*HOW MANY "UNUSED" PARAMETERS?	number of unused parameters (Sect. VIII.A)
*IS DATA IN "STANDARD" ODF FORMAT?	Y or N (Sect. VI.C.1)
*How many RADIUS parameters are used?	number of radii (Sect. V.F)
*How many UNUSED parameters are there?	
HOW MANY VARIED PARAMETERS?	the total number of parameters which are "flagged" in the PARameter file
HOW MANY DATA POINTS?	the number of data points that the analyst wishes to analyse simultaneously

VIII.C. SAMORT: PLOT THE OR RESOLUTION FUNCTION

When using the realistic resolution function (see Section IV.E) it may be useful to plot both the individual components of the resolution function and the final composite function. This can be accomplished using program SAMORT, which requires only the PARameter file and three other numbers (energy, mass, and flight path length) as input. Output consists of one ASCII file, as many as five plot (ODF) files, and as many as five additional ASCII files. The first ASCII file gives details of the case being run, including for example centroids for each component of the resolution function. Four plot files give time vs. resolution function for each component, and the fifth gives energy, resolution function, and time for the composite function (so that one can plot the resolution as a function of either energy or time). As with other plot files produced by SAMMY, these are in ODF format. For the benefit of SAMMY users who do not have the ORNL plotting package FORODF, the same information in the ODF files is also given in ASCII files with extension "PLT".

A sample interactive (unix) run of program SAMORT is accomplished with the following lines of input:

```
samort
a.par
180000.,57.935,201.578
```

where the energy at which the functions are to be evaluated is 180000 eV, the mass of the sample is 57.935 amu, and the flight path length is 201.578 meters.

The file a.par can be either the complete PARameter file, or may contain only the ORRES portion thereof. The file may look similar to the following:

```
ORRES
BURST 1          1.775     .5
TANTA 1          0.200       0.1
TANTA 1111       01.00      05.00      09.00      04.00.
TANTA            0.005       .005      0.005      0.005
TANTA 11         0.079      1.000
TANTA            0.04        0.5
LITHI 111        5.000   0.392235      1.009
LITHI            2.000   0.200000      0.500
CHANN 1     200000.000      7.179      4.000
```

(See Card Set 9 of the PARameter file, Table VIB.1, for interpretation of these numbers.)

Output plot files are as follows: The file SAM_ORR.ODF contains energies in Section 1, resolution function in Section 2, and time of flight in Section 3. File SAM_ORR_BURST.ODF contains time of flight in Section 1, and the burst-width component of the resolution function in Section 2. File SAM_ORR_TANTA.ODF contains time in Section 1 and the tantalum target component of the resolution function in Section 2. File SAM_ORR_CHANN.ODF contains

time in Section 1 and channel-width component in Section 2. Finally, the file SAM_ORR_LITHI.ODF contains time in Section 1 and the Lithium-glass detector resolution function in Section 2.

If the water moderator or the NE110 detector had been used instead, the respective file names would be SAM_ORR_WATER.ODF and SAM_ORR_NE110.ODF.

For a description of the contents of the ASCII PLT files, substitute "column" for "section" in the above description.

What follows is the output ASCII file SAMMY.ORR produced by running the example described above:

```
p ----------------------------
          1.7750E-03
a, w, x1, x2, x3, x0, alpha --
           1174.       463.6      1.7041E-04  8.5204E-04  1.5337E-03
          6.8163E-04   1.000
c ----------------------------
          7.1790E-03
d, f, g ----------------------
          5.0000E-03   392.2        1.009

<t>, t1, t2, t3, t4 ----------
         1.0894E-02  8.8750E-04  2.2220E-03  3.5895E-03  4.1951E-03
tlow, time, tup --------------
           34.253590       34.350633       34.361527
eup , em  , elow -------------
           181033.71       180000.00       179887.66
##########################
```

VIII.F SAMPLT: ALTERNATIVE FORM FOR PLOT FILES

Plotting with SAMMY has traditionally been accomplished by means of a set of utility programs FORODF [JC78]. SAMMY produces "ODF" or "plot" files containing the information (such as energies and cross sections) from which plots may be made using FORODF. (See, e.g., Section VII.C.) An alternative plotting program RSAP [RS01] is currently under development and will be made available at a future time.

Users on other systems may prefer to use other plotting packages. To facilitate this, the "SAMMY manager" can now choose between two alternatives when linking the program. To use the ODF option, the manager includes file modfio.o (compiled form of modfio.f) when linking those segments which require the plotting routines. To use the other option, the manager replaces file modfio.o with modf3.o (compiled form of modf3.f); this is most readily accomplished by simply renaming modf3.o to modfio.o prior to the link step. With this option, SAMMY will produce a "generic" binary file (also named SAMMY.ODF) which contains the same information normally stored in the ODF file, but in a form which can easily be read by a simple FORTRAN code.

A sample code SAMPLT (file mplt.f) is provided with the SAMMY FORTRAN. SAMPLT reads the binary file and produces an ASCII file (ASCII.PLT) which contains the same information as the ODF file on the ORNL version. The local SAMMY manager may wish to modify the file mplt.f to accommodate his system's needs; mplt.f contains extensive comment cards to aid in making the needed modifications.

Note that versions of this program (SAMPLT) prior to SAMMY-M5 were named "sambin" instead of "samplt". However, the word "bin" has special meaning on Unix systems; hence the name has been changed to avoid potential conflict with system routines.

VIII.G SAMTHN: THINNING DATA

Often a data file will contain more points than are needed to define the measurement (e.g., data appear to be very dense in energy regions where there is little structure in the data). SAMMY runs will therefore require far more computer time than is actually needed. For these reasons it is often deemed reasonable to "thin" the data, at least for preliminary runs. A program SAMTHN has been written for this purpose; it has not, however, been studied extensively so use with caution! Please note, also, that any results obtained with thinned data should ultimately be tested against the complete dense data set, to ensure that no important features were missed.

In running SAMTHN, the user provides two files, plus the name for the new thinned data file. The first user-provided file gives instructions on how the thinning should be done; the second is the dense data file. The first line of the thinning file contains three numbers (*N,Emin,Emax*) in I5, 2F10.1 format. The integer *N* tells how many data points are to be averaged together in the energy range from *Emin* to *Emax*. Second and subsequent lines contain two numbers (*N,Emax*); *Emin* is assumed to be equal to the previous *Emax*. Note that energies must be given from low to high, no matter what the ordering of data points in the original dense data file.

The fourth line of input (after the three file names) contains one character, which describes the type of input data in the dense file: O = Original (three energy-points per line, as in the original MULTI-style data format), C = CSISRS data, T = Twenty format, and D = Differential elastic data (ASCII format only). For differential elastic data, there is one additional line of input, an integer equal to the number of angles.

For O, C, or T, the format for the output thinned data file is always (3F20.10); in using this data file for SAMMY runs, the INPut file must contain the line USE TWENTY SIGNIFICANT DIGITS FOR EXPERImental data. For D, the output format is (F10.2,7F10.5); if this format is inappropriate, for this simple code the author assumes the user can make the necessary changes him/herself.

The algorithms used by SAMTHN to average the data are as follows:

$$\bar{E} = \left(\frac{1}{N} \sum_{i=1}^{N} \frac{1}{\sqrt{E_i}} \right)^{-2} , \qquad \text{(VIII.G.1)}$$

$$\bar{D} = \frac{1}{\bar{V}} \sum_{i=1}^{N} \frac{D_i}{V_i} , \qquad \text{(VIII.G.2)}$$

with

$$\bar{V} = \left(\sum_{i=1}^{N} V_i^{-1} \right)^{-1} , \qquad \text{(VIII.G.3)}$$

in which E represents the energy, D the data, and V the variance (i.e., the square of the uncertainty). Quantities with subscripts are from the original dense data set, and quantities with bars represent the averaged values.

Test Case Tr72 has two examples for thinning data.

VIII.K SAMCPR: COMPARE RESULTS

Program SAMCPR is as an aide in comparing cross sections calculated by one computer code (e.g., NJOY [Rm82] or REFIT [MM89]) with those calculated by SAMMY. First, a no-Bayes SAMMY run is made, using the other code's calculations as the DATa file, and including the alphanumeric command "compare experiment to theory" in the INPut file. SAMMY generates a binary file SAM53.DAT, which can then be read by program SAMCPR to produce the ODF file SAMCPR.ODF.

The contents of the various sections output file SAMCPR.ODF are as follows:

S1 = energy
S2 = X = "data," which may be a calculation from another code
S3 = S = "theory," which is the SAMMY calculation
S4 = $X - S$
S5 = $(X - S) / S$
S6 = $(X - S) / S \times 10^3$
S7 = $(X - S) / S \times 10^4$
S8 = $(X - S) / S \times 10^5$
S9 = $(X - S) / S \times 10^6$
S10 = S5 adjusted for small cross sections
S11 = S10 $\times 10^3$
S12 = S10 $\times 10^4$
S13 = S10 $\times 10^5$
S14 = S10 $\times 10^6$

For Section 10, the quantity $(X - S) / S$ is replaced by 10^{-25} if both X and S are smaller than 0.0001. Thus the value S10 through S14 will be sizeable only when the cross sections themselves are reasonably large.

Note that early versions of this program were called SAMCMP. However, "cmp" is a special word on unix systems; hence, the name has been changed.

VIII.M SAMRPT: PLOT RPI RESOLUTION FUNCTION

To plot the components and the total RPI resolution function (see Section IV.G, page 92s) at a given energy, use program SAMRPT. Input to SAMRPT consists of two lines of information: The first is the name of the PARameter file. Alternatively, it could be the name of a file containing the RPI portion of the PARameter file; the header line ("RPI Resolution function") may or may not be present. The second line contains the energy in eV, mass in atomic mass units (amu), and flight-path-length in m, in 3F format (separated by commas or spaces); alternatively the same information may be given as the first line in the RPI file. [Default values for these three quantities are 150.0, 183.85, and 25.604 respectively.]

Output from a run of SAMRPT consists of one ASCII file, SAMMY.RPI, which gives derived quantities such as the time-width associated with each component of the resolution function, as many as four plot (ODF) files plus four additional ASCII files:

SAM_RPI.ODF – S1 = energy, S2 = (total) resolution function, S3 = time
SAM_RPI_BURST.ODF – S1 = time, S2 = burst-width component
SAM_RPI_TDXXX.ODF – S1 = time, S2 = target-plus-detector component
SAM_RPI_CHANN.ODF – S1 = time, S2 = channel-width component

The four ASCII files have similar names to the four ODF files, with extension "ODF" replaced by "PLT". The same information from the various sections of the ODF files is given in the corresponding columns of the PLT files.

Test case TR53 gives numerous examples (not all of which make physical sense!) for the use of this program.

VIII.N SAMDIS: STATISTICAL DISTRIBUTIONS

The code SAMDIS a slightly-modified version of the code SAMDIST [LL95], which is used to verify the consistency of a resonance parameter set with the predicted theoretical statistical distribution. Three different tests can be performed:

1. Level spacing distributions are compared with the Wigner distribution law.
2. Neutron, radiation, and fission width distributions are calculated and compared with the χ^2 distribution with the appropriate number of degrees of freedom (dof = 1 for the Porter-Thomas distribution of neutron widths, dof = 2 or 3 for fission, and dof = ∞ for capture widths).
3. Long-range correlations of the energies are tested via the Δ_3 statistic of Mehta and Dyson.

Details of the three tests are given in the SAMDIST manual.

One modification to the code (and to the input; see Table VIIIN.1) has been made subsequent to the publication of the SAMDIST manual: The calculation of distribution of neutron widths now includes penetrabilities. Hence it is necessary to define the orbital angular momentum and to give the atomic mass of the target nucleus.

Table VIIIN.1. Input for program SAMDIS

Card Number	SAMDIST prompt	Response	Notes
1	Type d (for spacing), w (for width), or d3 (for delta3)	"d", "w", or "d3"	Line 3 appears only for "w" in line 1
2	Parameter file name	name of file	30 characters or less
3 ("w" only)	Enter particle channel	"neutron", "fission", or "gamma"	only lower case is permitted; note also that this line appears only for Test 2 ("w" in line 1)
4	Spin group, initial and final energies	SAMMY spin group number, Emin and Emax	free format, separate by commas
5 ("w" and "neutron" only)	Enter l and awr	integer value of orbital angular momentum, mass of target nucleus	This line is absent unless line 1 is "w" and line 3 is "neutron"
6 ("d" or "w" only)	Bin width for sampling	in units of energy	This line is absent for "d3"
7 ("w" only)	Degrees of freedom	degrees of freedom for chi-squared distribution	This line is here for "w" only (not for "d" or "d3")

VIII.O SAMSMC: MONTE CARLO MULTIPLE SCATTERING

In Sect. III.F, SAMMY's method of calculating the mutiple-scattering corrections to the capture and fission yields is presented. Because these calculations involve many complicated expressions as well as approximations whose legitimacy can be questioned, it is desirable to have an independent means of testing the calculations. Monte-Carlo is suitable for this task, as the method is completely different from the analytic-with-approximations approach taken in Sect. III.F.

The precursor to the code SAMSMC was written during the 1980's by Gerard de Saussure [GD80] and modified by Francis Perey. More recently, the SAMMY author has modified this code to include anisotropic scattering (non-s-waves) and more than one nuclide. In addition, an interface was developed with the SAMMY code, in order for SAMSMC to read and use the same Doppler-broadened cross sections and energies that are used in SAMMY.

Complete documentation of SAMMY's multiple-scattering capability, including comparisons to the Monte-Carlo results produced by SAMSMC, is in preparation [NL01]. What follows is preliminary documentation on the input to and use of SAMSMC.

1. Run SAMMY up to the point where it would begin execution of segment SAMSSM. (To do this, insert a line in the alphanumeric section of the INPut file which says
   stop_ssm__1
   in which there is one space after "stop" and two after "ssm". Alternatively, run SAMMY interactively and abort immediately when the code begins running SAMSSM.) The temporary file SAM51.DAT (SAM54.DAT if no Doppler) holds the cross sections needed for the multiple-scattering calculations. Rename this file to be used in later steps.

2. Run program SAMSMC (SAM-Ssm-Monte-Carlo), with the following input:
   a. Title [whatever you wish]
   b. Energy-mesh information [Emin,Emax,0.]
   c. Name of file with energy mesh [here only if Emin=0 in a]
   d. THSAMP, XSAMP, YSAMP, XBEAM, YBEAM [like Card Set 11 in INPut file for the regular SAMMY run]
   e. Thickness (in atoms/barn), Mass (in amu)
      where {Avagadro's #}$^{-1}$ is 1.6605402×10^{-24} grams/amu
   f. Maximum number of histories
   g. Number of scatterings to include
   h. Name of the file generated by SAMMY run [used to be SAM51.DAT]
   i. Maximum L-value in that file [where L is the vector sum of the orbital angular momentum for the individual levels]
   j. Normalize as yield (Y) or cross section (C) or other (O)

Two output files are produced by the SAMSMC run. MC_1.DAT holds the various cross sections, and MC_2.DAT contains results from 0 scattering, 1 scattering, two-or-more scatterings, and the sum of those three. Rename these, if desired.

3. Run program SAMSMX (SAMSMc-fiX), with the following input:
   a. Name of the cross section file produced by SAMSMC (MC_1.DAT)
   b. Name of the second file produced by SAMSMC (MC_2.DAT)

   Four output files are produced by this run. Three are ASCII files name MC_Y0.DAT, MC_Y1.DAT, and MC_Y2.DAT; these contain the self-shielded yield, the self-shielded plus single-scattering-corrected yield, and the full multiple-scattering-corrected yield, respectively. These files are in a form suitable for use as SAMMY DATa files, in the TWENTY format (see Sect. VI.C.1).

   The other output file produced by this procedure is named MC.ODF, and is an ODF file with the following sections:

   S1. energy in eV
   S2. 0 scattering (self-shielding) only
   S3. 1 scattering
   S4. 2 scatterings
   S5. 0 + 1
   S6. 0 + 1 + 2
   S7. capture cross section
   S8. total cross section
   S9. (1-exp(-th×total)) × capture / total

   Sections of this file can be compared to output in Section 4 of the ODF file produced by the corresponding SAMMY runs. For example, output from a SAMMY run which includes single scattering (finite disk) but not double scattering would be compared to Section 5 in MC.ODF.

XI. DESCRIPTION OF THE COMPUTER CODE SAMMY

The computer code SAMMY was originally developed for ease and efficiency of running on the DECSystem-10 (PDP-10) at the Oak Ridge Electron Linear Accelerator (ORELA). Because core storage rather than CPU time was the limiting factor on the PDP10, a number of techniques were used to preserve core, occasionally at the expense of runtime. These techniques include dynamic allocation of array storage (Section XI.A), use of temporary data files to store intermediate results (Section XI.B), and division of the program into substantially independent segments (Section XI.C).

In 1985 ORELA replaced its PDP10 with a VAX785, and SAMMY migrated to the system. Since the mid 1990's, the primarily operating system for SAMMY development has been UNIX, but portability to VMS operating systems has been maintained. Currently the author maintains the code under UNIX (f77 on IBM and VAX-Alpha workstations), VMS, and LINUX operating systems. The same version also works on Windows under Compaq FORTRAN.

Recently the "division of the program into substantially independent segments" was significantly altered; see Section XI.C for details. Future plans call for continued modernization of the coding, including conversion to FORTRAN 90; this will eliminate the archaic "dynamic allocation of array storage" currently in use (Section XI.B).

XI.A DYNAMIC ALLOCATION OF ARRAY STORAGE

Because SAMMY was developed prior to the advent of FORTRAN 90, which supports dynamic storage allocation, SAMMY uses its own scheme for dynamic allocation of array storage. Since this scheme is more cumbersome (and involves one fixed limit), this aspect of the code will be one of the first to be modernized when the code is converted to FORTRAN 90. What follows is a brief description of the scheme currently in use in SAMMY (Version M5 and earlier).

All arrays required by the computer program are stored in one location in COMMON/EXPAND/A(*n*), where *n* is a large number. (This common statement, in turn, is stored in the INCLUDE'd file B00ZYX.) Allocation of space in this common block is accomplished via a call to FUNCTION IDIMEN, which remembers the last location allocated, and appends the new array to that position. When an array is no longer needed, its space is released for future use via another call to IDIMEN. IDIMEN issues a warning if more than *n* words are required in COMMON/EXPAND/A, and also indicates the maximum size actually used in each segment of the program.

[The value for the dimension *n* is stored as variable MSIZE which is defined in the INCLUDE'd file BAAZYX and stored in COMMON/OOPS/; this common block is stored in the INCLUDE'd file B10ZYX.]

The SAMMY scheme for dynamic allocation of array storage is best illustrated with a simple example. Let us suppose that two vectors V1 and V2, both of length N, are to be initialized, added, and stored in V1, after which V2 is no longer required. A program to perform these operations is given in Table XIA.1. Notice that mnemonic names can be used in the usual manner in all subroutines, provided arrays are input to the subroutines through argument listings.

Historically there have been many advantages to using dynamic allocation of array storage. First, core requirements are kept to a minimum, since only the array length actually needed is allocated and temporary arrays are released when no longer needed. Secondly, because allocation is made during the execution of a program, substantial changes in the dimensions for a specific case do not require recompilation of the program. Finally, when recompilation is needed (when the maximum array space requirement is larger than *n*), only those routines containing COMMON/EXPAND/A need to be recompiled.

XI.B USE OF TEMPORARY DATA FILES TO STORE INTERMEDIATE RESULTS

Output to and input from temporary files is a time-honored method of saving core space at the expense of runtime. In versions of SAMMY prior to M5, the use of temporary files also provided the necessary linkage from one module to another; I/O for this purpose has now been eliminated, since the segments of the code are now united into one large code. Nevertheless there are still many temporary files created by a SAMMY run; many of these will also be phased out as modernization of the code proceeds. For now, upon successful completion of a SAMMY run, the temporary files may be deleted.

It is still possible to debug the code in a piece-wise fashion, one segment at a time. However, it now requires a bit more planning on the part of the programmer. First, a SAMMY run is made which includes the alphanumeric line

stop *xyz* *n*

in the INPut file, where *n* is a one-digit integer proceeded by two spaces, and *xyz* is the name of the segment for which debugging is needed. This line is a command to SAMMY to cease execution just prior to the beginning of the *n*th pass through segment *xyz*, and generate the temporary files that permit restart of that segment alone. After this run finishes, the programmer can save those temporary files and use them for debugging on segment sam*xyz*.

The temporary files generated by SAMMY are listed in Table XIB.1, along with input and output files required by or produced by the code. "Standard" names referenced in the third column of the table are "SAMxx.DAT," where xx is replaced by the unit number.

Table XIB.1. Files used by SAMMY. Note that the letter A, B, or O in the second column indicates whether the file is written as ASCII, binary, or ODF file

Unit No.	A, B, O	File name if not standard	Segment: subroutines in which this file is written	Segment: subroutines in which this file is read	Content
5	A	(From terminal, or batch file)		mas: inppar, fpar, sumstr, fixnam, datcov, writ16, file2x ort: samort rpt: samrpt rsl: samrsl sta: samsta thn: samthn	See Table VID.1
6	A	Log file	[Many places]		
10	A	ENDF/ B-VI file 2		mas: endfb6, rcontx, rcont, rtab1, rlist	See Table VIF.1
10	A	ENDF/B file 3		rec: read3, rdndf3 cro: read3, rdndf3 xct: read3, rdndf3	File 3 contribution to cross section
10	A	MXW file		mxw: rktxxx, readkt	See Section VI.H
10	A	NDF file		ndf: endfb6, rdndf, rdntgq	See Section VI.F
10	A	(No standard name)		thn: samthn	File with thinning instructions; see Section VIII.G
11	A	INPut file		mas: finp, new, newinp	See Tables VIA.1 and VIA.2
12	A	(No standard name)	thn: out		File containing thinned data in "twenty" format; see Section VIII.G.
12, 32	A	Initial PARa-meter file		mas: fpar inp: qresp, qfudge, qextr, qrext, qradi, qisot, qbroa, qmisc, qpmcs, qorre, qrpire, qnorm, qbackg, qdatp, qunus, qbaga, qcova, qrelu, qexpl, pread	See Table VIB.1

XI.C DIVISION OF THE PROGRAM INTO AUTONOMOUS SEGMENTS

Prior to version M5 of SAMMY (in the year 2000), the code SAMMY was actually a system of ~50 semi-autonomous codes which executed sequentially and which communicated with each other via I/O from/to temporary files. This structure was originally necessary, when computer memory was small and virtual memory non-existent, and it also had the great virtue of permitting the author to debug each segment independently of the others.

With the advent of modern computers, this independent nature of the segments became obsolete and has therefore been eliminated. The various pieces have been assembled into one code. Many (but not yet all) of the read and write operations have also been eliminated. Users will notice two immediate benefits from this modernization of the code:

(1) Porting SAMMY to a new platform is considerably easier than in the past. Subroutine execv, the C-language (or system) routine which permitted one FORTRAN routine to initiate execution of another, was a major source of difficulty in porting the program; execv is no longer used. Also, the location (path name) of the executable files must no longer be specified within the code prior to compilation.

(2) Execution time is shortened. The author has noted improvement by as much as 70% on the test cases, though more modest gains are likely on routine runs.

The basic structure of the code has not changed, however: SAMMY still consists of semi-independent segments which are now called sequentially by a main routine. There are approximately fifty segments (or modules), not all of which are used for every SAMMY run. Table XIC.1 describes the functions of each segment and indicates the calling sequence. The order of the segments in the table is alphabetical; a flow chart (at the end of the table) shows the order in which the modules are used.

By convention, the segment name is "sam*abc*" where *abc* is replaced by the three characters listed in the table. For most of the segments, relevant files are contained within a subdirectory of the same three-character name (in lower case, on UNIX operating systems). (Most segments also make use of subroutines in files stored in other subdirectories.) The name and location conventions are not, however, rigidly followed. Some subdirectories store files used in many segments, but do not themselves constitute a segment. Other subdirectories hold coding for several segments.

In addition to the segments that operate within a SAMMY run, a number of auxiliary programs are available to be used in conjunction with SAMMY. These programs are described in Section VIII; however, most are also included in Table XIC.1.

Table XIC.1. Segments of the code SAMMY

Segment	Alternative segments	Primary functions	Control passes to which segment?	Control comes from which segment?
ACS		Calculate cross sections etc. for unresolved resonance region	MPW	FFF, FIT
AMR		Reorganize covariance file when changing data-reduction parameters (Section VIII.A)	(Stand-alone program)	
ANG		Generate angular distribution (Section III.E)	INT, ORR, RPI, or RSL	INT, DBD, DOP, FGM, or XCT
AVG	GRP	Generate "multigroup cross sections", i.e., averages of theoretical and experimental cross sections (Section V.C)	DAT or END	SQU
BIN	PLT	(Renamed to PLT because BIN is a reserved name on some systems)		
BLK		(Subdirectory stores common blocks)		
COU	XXX	(Subdirectory contains routines used to generate Coulomb penetrabilities, shift factors, and hard sphere phase shifts)		
convrt		Main program for converting resonance parameters from REFIT format to SAMMY or v.v. Stored in subdirectory /ref/	INP, refsam	
CPR (formerly CMP)		Read binary file SAM53.DAT (which was generated by samnpv or samipq) and create ODF file	(Stand-alone program samcpr)	
CRO	MLB, XCT	Generate theoretical cross sections using the Reich-Moore approximation to multilevel R-matrix theory (Section III.A)	DBD, DOP, FGM, INT, MXW, NTG, ORR, RPI, RSL, or SQU	THE
DAT		Read the DATa file; generate the auxiliary energy grid used for broadening	IDC, REF, or THE	AVG, FIN, NEW, or OLD

Table XIC.1 (continued)

Segment	Alternative segments	Primary functions	Control passes to which segment?	Control comes from which segment?
DAX	DAT	(eliminated with version M5)		
DBD	DOP, FGM	Doppler-broaden the theoretical cross section using the original method. (Section IV.A.1)	ANG, INT, ORR, RPI, RSL, or SSM	CRO, INT, MLB, or XCT
DIS		Calculate statistical properties	(Stand-alone program samdis)	
DOP	DBD, FGM	Doppler-broaden the theoretical cross section using the Leal-Hwang method (See Sect. IV.D)	ANG, INT, ORR, RPI, RSL, or SSM	CRO, INT, MLB, or XCT
END		Reorganize files for another pass, or delete temporary files at end of run. Subdirectory also contains files with output subroutines	INP or quit	AVG, FIN, GRP, MAS, MXW, NDF, ODF, or REC, RST, YWY
FDC		Update data file with implicit data covariance information	(ends)	INP
FFF		Read input for analysis of unresolved resonance region	ACS	MAS
FGM	DBD, DOP	Doppler-broaden via the free gas model (Section IV.F)	ANG, INT, NTG, ORR, RPI, RSL, SQU, or SSM	CRO, MLB, XCT
FIN		Convert results from *u*-parameters to physical parameters; output results	DAT, END, or THE	IPQ, MPW, or NPV
FIT		Output results for unresolved resonance region	ACS	MPW
FNC		(Subdirectory contains coding for frequently used functions)		
GRP	AVG	Generate multigroup cross sections using Bondarenko narrow-resonance weighting scheme (Section V.C.2)	END	SQU
IDC		Read and sort implicit data covariance information	REF, RST, THE	DAT

Table XIC.1 (continued)

Segment	Alternative segments	Primary functions	Control passes to which segment?	Control comes from which segment?
INP		Read INPut file for control commands and for information about the data set; read through PARameter file to set array sizes	FDC, PAR	END or MAS
INT		Print theoretical cross sections and/or partial derivatives; write parts of plot file	ANG, DBD, DOP, FGM, MXW, NPV, NTG, ORR, RPI, RSL, SQU, SSM, WYW, or YWY	ANG, CRO, DBD, DOP, FGM, MLB, ORR, RPI, RSL, SSM, or XCT
IPQ	MPW, NPV	Solve IPQ form of Bayes' Equations (See Sect. II.B.1.b)	FIN	SQU
MAS		Read input commands and file names; read portions of INPut file; organize the manner in which SAMMY will run	END, FFF, INP, or ODF	SAMMY
MLB	CRO, XCT	Generate theoretical cross sections using the single or multilevel Breit-Wigner theory (Section III.C)	DBD, DOP, FGM, INT, MXW, NTG, ORR, RPI, RSL, or SQU	THE
MPW	IPQ, NPV	Solve Bayes' Equations via the MPW method (See Sect. II)	FIT	ACS, SQU, WYW
MXW		Generate stellar (Maxwellian) average capture cross section (Section V.P)	END	CRO, MLB, REC, SQU, or XCT
NDF		Output resolved resonance parameters in ENDF-6 file 2 format	END	NEW or OLD
NEW	OLD	Generate the initial covariance matrix for the parameters	DAT, NDF, REC, REF, WYW	PAR
NPV	IPQ, MPW	Solve NPV form of Bayes' Equations (See Section II.B.1.a)	FIN	INT, NTG, or SQU

Table XIC.1 (continued)

Segment	Alternative segments	Primary functions	Control passes to which segment?	Control comes from which segment?
NTG		Calculate integral quantities (see Sect. V.I)	NPV	CRO, FGM, MLB, REC, SQU, or XCT
ODF		Initialize the plot (ODF) output file by writing energies into S1, data into S2 and S6, and uncertainties into S3 and S7	END	MAS
OLD	NEW	Read the initial covariance matrix for the parameters from a binary file generated by an earlier SAMMY run	DAT, NDF, or REC	PAR
ORR	RPI, RSL	Resolution-broaden the theoretical cross section using the realistic resolution broadening (Section IV.E)	INT	ANG, CRO, DBD, DOP, FGM, INT, MLB, SSM, or XCT
ORT		(Stand-alone program to study ORR resolution function)		
PAR		Read parameters from PARameter file	NEW or OLD	INP
PLT		Convert from binary plot file to another option	(Stand-alone program samplt)	
QUA		(Stand-alone program to generate quantum numbers)		
REC		Reconstruct point-wise cross section from resonance parameters	END, MXW, or NTG	NEW or OLD
REF		Convert resonance parameters from SAMMY to REFIT format; a part of program convrt (not program sammy)		DAT, IDC
refsam		Convert resonance parameters from REFIT to SAMMY format; a part of program convrt; files in subdirectory /ref/	WRT	convrt

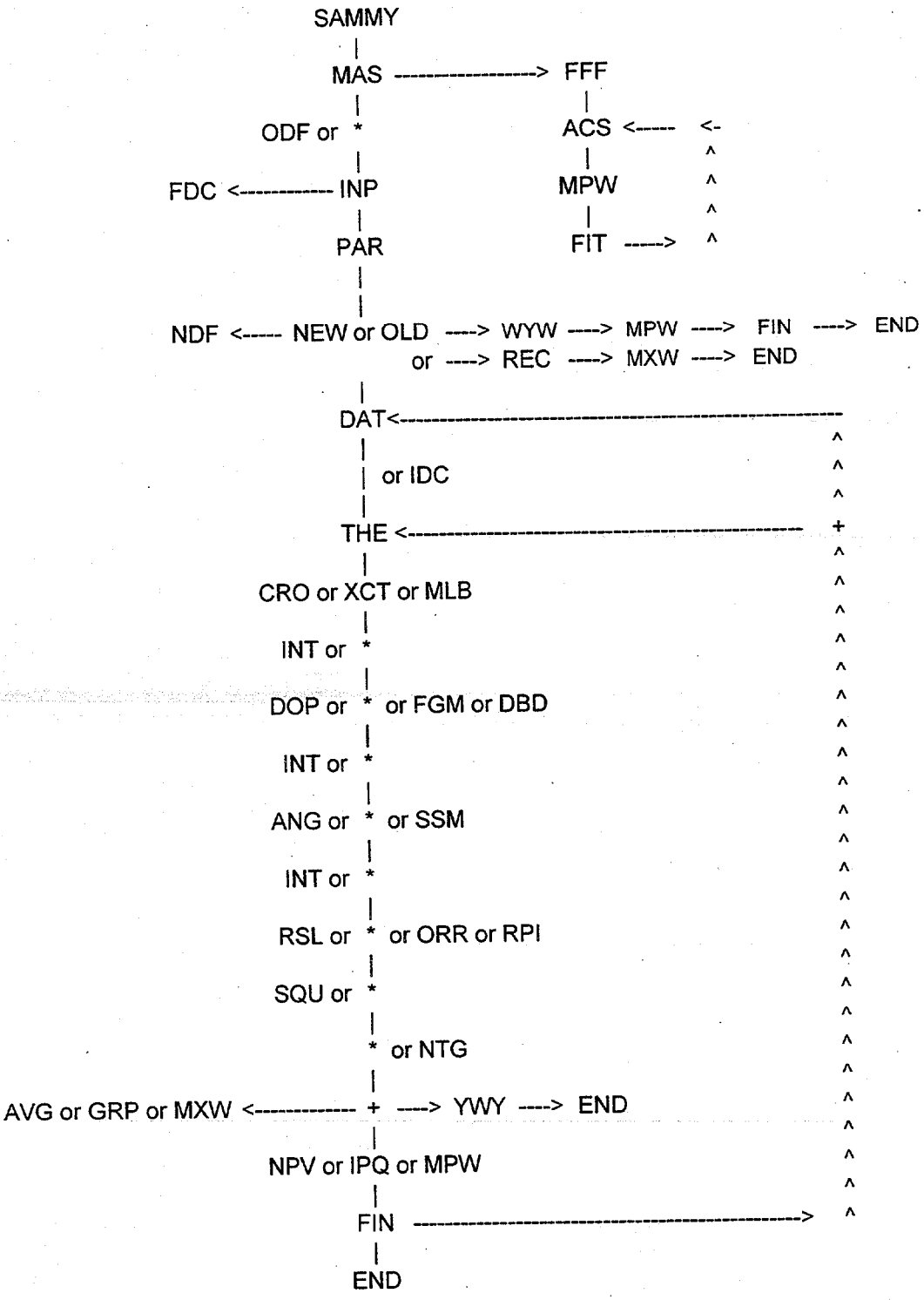
Table XIC.1 (continued)

Segment	Alternative segments	Primary functions	Control passes to which segment?	Control comes from which segment?
refwrt		Output resonance parameters from in REFIT format after conversion from SAMMY format; a part of program convrt; files in subdirectory /ref/	(ends)	REF
RPI	ORR, RSL	Resolution-broaden the theoretical cross section using the RPI resolution function	INT	ANG, CRO, DBD, DOP, FGM, INT, MLB, SSM, or XCT
RPT		(Stand-alone program to study RPI resolution function)		
RSL	ORR, RPI	Resolution-broaden theoretical cross section using the original method (Section IV.A.2)	INT	ANG, CRO, DBD, DOP, FGM, INT, MLB, SSM, or XCT
RST		(Stand-alone program to study RSL resolution function)		
SAMMY		Begin	MAS	
SMC		Generate multiple-scattering correction to capture or fission yields via Monte-Carlo method	stand-alone program samsmc	
SQU		Expand the triangular storage of the covariance matrix to full square form	AVG, IPQ, MPW, MXW, NTG, or NPV	CRO, INT, MLB, or XCT
SSM		Perform self-shielding and multiple-scattering calculation for capture yields	INT, ORR, RPI, or RSL	DBD, DOP, FGM, INT, or XCT
STA		(Sand-alone program samsta to generate stair-case plots)		
THE		Perform bookkeeping related to cross-section calculations	CRO, MLB, or XCT	DAT, FIN, IDC
THN		(Sand-alone program to thin dense data)		

Table XIC.1 (continued)

Segment	Alternative segments	Primary functions	Control passes to which segment?	Control comes from which segment?
WRT		Output SAMMY-style resonance parameters after conversion from REFIT format; a part of program convert; stored in subdirectory /ref /	(ends)	refsam
WYW		Read Y_i and W_i and add, for use in segment MPW (see Sect. II.B.1.c)	MPW	NEW, OLD
XCT	CRO, MLB	Generate theoretical cross sections using alternative formulation of Reich-Moore (Section III.D)	ANG, DBD, DOP, FGM, INT, MXW, NTG, ORR, RPI, RSL, SQU, or SSM	THE
XXX		(Subdirectory stores routines relating to penetrabilities, shift factors, and hard-sphere phase shifts for non-Coulomb interactions)		
YWY		Generate Y_i and W_i, for use in segment MPW (see Sect. II.B.1.c)	END	INT, NTG, SQU

Fig. XIC.1. Flow chart for SAMMY.



XI.D QUALITY ASSURANCE

The SAMMY quality assurance program involves a series of "test cases," each of which is designed to test a particular feature of the code. Whenever a new feature is added to SAMMY or a major bug exterminated, a new test case is developed. Prior to the release of a new version of the code, all test cases are run on several computer platforms, to ensure that recent changes have not adversely affected the behavior of older features. These test cases, both input and output, are released, along with the source codes (e.g., from RSICC); anyone wishing to port SAMMY to his or her own computer is advised to run a significant number of test cases, compare output, and resolve major differences before beginning new analyses. In particular, a user should run those test cases which contain the features s/he uses in her/his own research.

Table XID.1 gives a brief description of the test cases, which are numbered chronologically in order of their development. Cases 1 through 9 are labeled "tr1" through "tr9" (where "tr" denotes "trial" number), and cases 10 through 99 are "t10" through "t99." These labels are the first three characters of most files relating to these test cases; in addition each test case is in a separate subdirectory. In each case, the command file is named "m1t*xx*" where *xx* is either r1 through r9, or *xx* is the two-digit trial number. [And, since there are now 99 test cases, that convention will be modified in the near future.]

Note that some numbers (e.g., tr33) are omitted from the listing in Table XID.1 and are not included in the release. Note also that all experimental data used in the test cases are to be treated as "dummy" data, not to be used for any purpose other than to verify the accuracy of the SAMMY calculations. The same is true of resonance parameters used in the test cases.

Table XID.1. SAMMY test cases

No.	Module tested	Main feature being tested	Data type	Nuclide
1	samdat	Correlated data (DCV file)	Elastic	Ni60
2	samipq, samnpv	Comparison of different solution methods for Bayes' equations	Trans-mission	P204
3	sampar	R-external	Trans	Ni60
4	samfin, samold	Simultaneous vs sequential solution of Bayes' equations	Trans	Ni60
5	samdat	Use ODF file as input	Fission	Am241
6		Resonance parameters only	Trans	Ni60
7	samamr	Rearranging "active" data-reduction parameters	Trans	Fe56
8	samdat	Comparing alternative auxiliary grids	Trans	Ni58
9		Simultaneous vs sequential solution of Bayes' Equations; explicit input of prior uncertainties	Fission	Pu239
10	saminp	New spin group format	Trans	Zr93
11		R-external	Trans	Fe54
12		Varying channel radius, normalization, and/or background	Trans	Ni58
13	samxct	Channel radius	Trans	Ni58
14	samavg	Averaging experimental and theoretical data	Fissi	Pu239
15	samnew	"Relative uncertainties" vs "explicit uncertainties" in PARameter file	Trans	Ni58
16		Radius	Trans	Ni58
17		Long run	Fission	Pu239
18		Different cross sections	(All)	U235
20	samfgm, samdbd, samdop	Different versions of Doppler broadening	Fission	U235
21	samorr	Oak Ridge Resolution function; vary radius	Trans	Ni58
22	samrsl	Shift exponential tail on resolution function	Trans	Fe56

Table XID.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
23	samndf	Make ENDF File 2	Trans	P204, Ni58
24		Vary radii	Trans	Natural Fe
25	sammlb	MLBW vs RM	Trans	Fe56
26	samfgm	Compare different Doppler broadening methods	Fission	Am241
27		Generate partial derivatives	Fission	U235
28	samdbd	No low-energy Doppler broadening	Total	Pu241
29		Abundance as a variable	Trans	Ni58
30		Remove resonances using negative group number in PARameter file	Trans	Ni58
31	samdop	LH vs no broadening vs FGM at thermal	Fission	U235
32	samamr	Vary radii, convert "active" data-reduction parameters	Trans	Fe56
34	samorr	ORR resolution function at thermal energies	Trans	Cu65
35		Γ_γ as miscellaneous parmameter	Capture	U235
37	samrec	Reconstruct point-wise cross sections from resonance parameters	All	lots
39	samssm	Self-shielding and multiple-scattering corrections to capture yields	Capture	Ni58
42	sammxw	Maxwellian (stellar) averages	Capture	Ni58
43	samang	Differential elastic angular distributions	$d\sigma / d\Omega$	Ni58,Cr52,..
45	samssm	Multiple-scattering with more than one nuclide in sample	Capture	Natural Fe
46	samssm	Ditto, making plots with and without corrections	Capture	Natural Fe
47		Vary tzero and eLzero	Trans	Fe56
48	samrsl	Channel resolution varies with energy	Fission	Pu239
49	samrec, sammxw	Reconstruct point-wise cross sections, use results to calculate stellar averages	Capture	Fe54
50	sammas	Use ENDF File2 for input to SAMMY	Trans	Co59

Table XID.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
51	sammxw	Various ways to generate stellar averages	Capture	Ba136
52	samssm	Self-shielding and multiple-scattering corrections	Capture	Ba134
53	samrpt	Generate RPI resolution function		
54	samrpi	Use RPI resolution function	Trans	W
55		Paramagnetic cross section	Total	Dummy
56		Background function		Dummy
57	samssm	Self-indication data	Self-ind	Dummy
58	samdop, samfgm	Very low energy Doppler	Capture	Dummy
60	samssm	Self-shielding and multiple-scatter	Capture	Ba136
61	samref	Convert REFIT input to SAMMY and vv		
62	samssm	Double (etc.) scattering	Capture	W
63		Constant cross section		Dummy
64		Fission yields, polar coordinanants,	Fission	U235
67	samdat	Twenty significant digits for data		Dummy
69	samntg	Integral quantities	All	U235
70	samidc, samfdc	Implicit data covariances		U235
71		Write covariance matrix in compact ASCII format		
72	samthn	Thinning data		
73	samfff	Unresolved Resonance Region	many	U235
74	samidc	Various ways to use data covariance information		
75	samavg	Generate group average cross sections with and without covariances		
76		Like tr39 but uncorrected	Capture	Ni58
77	samxct, samntg	Comparison with other codes	(All)	U235
78	samxct	Spin-group-dependent detector efficiencies	Capture	Ba136
79	samrsl	Energy-dependent exponential broadening	Capture	Ba136

Table XID.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
80	samrsl	Exponential folding width	Total	U235
81	samrsl	Energy-dependent exponential folding width	Total	U235
82	samywy, samwyw	Retroactive covariance	many	U235
83	samold, samgrp	Concise covariance format; Bondarenko multi-group cross sections	many	U235
84	samold	Concise covariance format	capture	U235
85	samgrp	Bondarenko averaging	capture, total	U235, Al27
86	samndf	Generate and/or read-and-use ENDF file 2	trans, capture	Al27
87	samamr	background functions and RPI resolution function	trans	W183
88	samfff, samacs	unresolved resonance region with many data sets, each with its own normalization	many	Cm244
89	samywy, samwyw	retroactive covariance matrix; covariance for multigroup cross sections	total	Si29
91	samxct	Coulomb	(n,α)	O16
92	samdis	Luiz Leal's samdis (samdist) program		
93	samxct	Exit channels specified separately	reaction	O16
94	samrpi, samrpt	RPI resolution function	trans	Tc99
95	samrpt	RPI resolution function		Tc
96	samsmc	Monte Carlo generation of multilple-scattering corrections to capture yield	capture	Ni58
99	samorr, samfgm	general	capture	Pt192

REFERENCES

AB82 A. R. Barnett, *Comp. Phys. Comm.*, **27**, 147 (1982); *Comp. Phys. Comm.*, **21**, 297 (1981)

AF71 Anthony Foderaro, *The Elements of Neutron Interaction Theory*, MIT Press, 1971.

AG65 A. Gilbert and A. G. W. Cameron, *Can. J. Phys.*, **43**, 1446 (1965).

AG73 A. Gandini, *Nuclear Data and Integral Measurements Correlations for Fast Reactors*, Part I and II, Comitato Nazionale Energia Nucleare, Casaccia, Italy, 1973, RT/FI(73)5 and 22 (1973).

AL58 A. M. Lane and R. G. Thomas, *Rev. Mod. Phys.* **30**, 257 (1958).

BM96 Brian E Moretti, *Molybdenum Neutron Transmission Measurements and the Development of an Enhanced Resolution Neutron Target*, Ph.D. Thesis in Nucl. Engineering & Science, Rensselaer Polytechnic Institute, Troy NY, August 1996.

CC83 C. Coceva, R. Simonini, and D. K. Olsen, "Calculaton of the ORELA Neutron Moderator Spectrum and Resolution Function," *Nucl. Inst. Meth.* **211**, 459 (1983).

CP84 C. M. Perey, Oak Ridge National Laboratory, personal communication

CP88 C. M. Perey, F. G. Perey, J. A. Harvey, N. W. Hill, N. M. Larson, and R. L. Macklin, *^{58}Ni + n Transmission, Differential Elastic Scattering and Capture Measurements and Analysis from 5 to 813 keV*, ORNL/TM-10841, ENDF-347, Oak Ridge National Laboratory, 1988.

CR58 C. W. Reich and M. S. Moore, *Phys. Rev.* **111**, 929 (1958).

DH53 D. L. Hill and J. A. Wheeler, *Phys. Rev.* **89**, 1102 (1953).

DL83 D. C. Larson, N. M. Larson, J. A. Harvey, N. W. Hill, and C. H. Johnson, *Application of New Techniques to ORELA Neutron Transmission Measurements and their Uncertainty Analysis: the Case of Natural Nickel from 2 keV to 20 MeV*, ORNL/TM-8203, ENDF-333, Oak Ridge National Laboratory, October 1983.

DL84 D. C. Larson, N. M. Larson, and J. A. Harvey, *ORELA Flight Path 1: Determinations of Its Effective Length vs Energy, Experimental Energies, and Energy Resolution Function and Their Uncertainties*, ORNL/TM-8880, Oak Ridge National Laboratory, June 1984.

ENDF-102 *ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF-6*, written by the Members of the Cross Section Evaluation Working Group, ed. V. McLane, C. L. Dunford, P. F. Rose, BNL-NCS-4495, Brookhaven National Laboratory, November 1995.

ENDF99 *Summary of the 48th Cross Section Evaluation Working Group Meeting*,, Brookhaven National Laboratory, November 1999, Attachment 3-5.

EV58 E. Vogt, *Phys. Rev.* **112** (1958) 203.

EW47 E. P. Wigner and L. Eisenbug, *Phys. Rev.* **72** (1947) 29.

FF80 F. H. Froehner, *Applied Neutron Resonance Theory*, reprinted from *Nuclear Theory for Applications*, p. 59 ff., International Centre for Theoretical Physics, Trieste (1980). Available as KFK 2669 (1978). See also "Applied Theory of Resolved and Unresolved Resonances," *Applied Nuclear Theory and Nuclear Model Calculations for Nuclear Technology Applications*, M. K. Mehta and J. J. Schmidt, eds., World Scientific, Singapore, 1989, p. 170.

FF83 F. H. Froehner, B. Goel, and U. Fischer, "Calculation of Average on Capture Cross Sections for Actinides — Level-Statisical vs Globalon Approach,", *Proc. Mtg. Fast Neutron Capture Cross Sections*, Argonne, Illinois, April 20-23, 1982, ANL-83-4, p. 116, Argonne National Laboratory (1983).

FF89 F. H. Froehner,"Evaluation of the Unresolved Resonance Range of ^{238}U," *Nucl. Sci. Eng.* **103**, 119 – 128 (1989).

FF99 F. H. Froehner, personal communication (1999)

FG00 F. Gunsing, Saclay, personal communication (2000)

FP84 F. G. Perey, ORNL, personal communication (1984)

FP89 F. G. Perey, ORNL, personal communication (1989)

FP89a F. G. Perey, *RFUNC -- A code to Analyze Differential Elastic-Scattering Data*, ORNL/TM-11112, Oak Ridge National Laboratory, March 1989.

FP92 F. G. Perey, ORNL, personal communication

GA74 George F. Auchampaugh, *MULTI, A FORTRAN Code for Least-Squares Shape Fitting of Neutron Cross-Section Data Using the Reich-Moore Multilevel Formalism*, LA-5473-MS, Los Alamos Scientific Laboratory, 1974.

GD78 G. deSaussure, D. K. Olsen, R. B. Perez, *SIOB: A FORTRAN Code for Least-Squares Shape Fitting Several Neutron Transmission Measurements Using the Breit-Wigner Multilevel Formula*, ORNL/TM-6286, ENDF-261, Oak Ridge National Laboratory, 1978.

GD80 G. deSaussure and F. G. Perey, ORNL, personal communication.

GD84 G. deSaussure, ORNL, personal communication.

HD97 H. Derrien, N. M. Larson, and L. C. Leal, *Covariance Matrices for Use in Criticality Safety Predictability Studies*, ORNL/TM-13492, Oak Ridge National Laboratory, September 1997.

HD00 H. Derrien, ORNL, personal communication.

IB64 I. I. Bondarenko, ed., *Group Constants for Nuclear Reactor Calculations*, Consultant Bureau, New York, 1964.

JB52 J. M. Blatt and L. C. Biedenharn, "The Angular Distribution of Scattering and Reaction Cross Sections," *Rev. Mod. Phy.* **24**, 258 (1952).

JC78 J. G. Craven, *OPRODF, A DECsystem-10 Data Manipulation Program for ORELA Data Formatted Files*, ORNL/CSD/TM-45, Oak Ridge National Laboratory, May 1978.

JD79 J. J. Dongarra, C. B. Moler, J. R. Bunch, G. W. Stewart, *LINPACK User's Guide*, SIAM (1979).

JM80 J. H. Marable, C. R. Weisbin, and G. deSaussure, "Combination of Differential and Integral Data" in *Sensitivity and Uncertainty Analysis of Reactor Performance Parameters, Adv. Nucl. Sci. and Technology*, Plenum Press, New York, Martin Becker, ed., 1980.

KC53 K. M. Case, F. de Hoffman, and G. Placzek, *Introduction to the Theory of Neutron Diffusion*, Los Alamos Scientific Laboratory, 1953.

KW84 K. Wisshak, F. Kappeler, G. Reffo, and F. Fabbri, "Neutron Capture in *s*-Wave Resonances of Iron-56, Nickel-58, and Nickel-60," *Nucl. Sci. Eng.* **86**, 168 (1984).

LL85 L.C. Leal, ORNL, personal communication, 1985

LL95 L. C. Leal and N. M. Larson, *SAMDIST, A Computer Code for Calculating Statistical Distributions for R-Matrix Resonance Parameters*, ORNL/TM-13092, Oak Ridge National Laboratory, September 1995.

LL96 L. C. Leal and N. M. Larson, in preparation.

LL98 L. C. Leal, R. O. Sayer, N. M. Larson, and R. R. Spencer, "R-Matrix Evaluation of 16O Neutron Cross Sections up to 6.3 MeV," ANS Winter Meeting, Washington, D. C., Nov. 16-20, 1998.

MM64 M. D. Mintz and D. P. Jordan, *A 'Progressive' Interpolation Scheme for Hand and Digital Computer Analysis of Tabulated Data*, Report UCRL-7681, Lawrence Livermore Laboratory, 1964.

MM89 M. C. Moxon, "REFIT2: A Least Squares Fitting Program for Resonance Analysis of Neutron Transmission and Capture Data," NEA-0914/02, July 1989.

NAG Numerical Algorithms Group (USA) Inc., 1250 Grace Court, Downers Grove, Illinois 60516, USA.

NL80 N. M. Larson and F. G. Perey, *User's Guide for SAMMY: A Computer Model for Multilevel R-matrix Fits to Neutron Data Using Bayes' Equations*, ORNL/TM-7485, ENDF-297, Oak Ridge National Laboratory, November 1980.

NL82 N. M. Larson, *User's Guide for BAYES: A General-Purpose Computer Code for Fitting a Functional Form to Experimental Data*, ORNL/TM-8185, ENDF-323, Oak Ridge National Laboratory, August 1982.

NL84 N. M. Larson, *User's Guide for ALEX: Uncertainty Propagation from Raw Data to Final Results for ORELA Transmission Measurements*, ORNL/TM-8676, ENDF-332, Oak Ridge National Laboratory, February 1984.

NL89 N. M. Larson, D. C. Larson, C. M. Perey, and F. G. Perey, *LEVDEN: A Level Density Code Using the Fermi-Gas Model*, ORNL/TM-10843, in preparation.

NL97 N. M. Larson, L. C. Leal, H. Derrien, *Integral Data Analysis for Resonance Parameters Determination*, ORNL/TM-13495, Oak Ridge National Laboratory, September 1997. Also *Nucl. Sci. and Eng.* **131** 254 (February 1999).

NL98 N. M. Larson, M. C. Moxon, L. C. Leal, and H. Derrien, *Doppler Broadening Revisited*, ORNL/TM-13525, Oak Ridge National Laboratory, 1998.

NL98a N. M. Larson, "Introduction to the Theory and Analysis of Resolved (and Unresolved) Neutron Resonances via SAMMY," Proceedings the IAEA Workshop on "Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety" held at the International Centre for Theoretical Physics, Trieste, Italy, 23 February - 27 March 1998, published by World Scientific, 1999. Also published as ORNL/M-6576, July 1998.

NL98b N. M. Larson, L. C. Leal, and H. Derrien, "Efficient Use of Bayes' Equations for Fitting Neutron-Induced Cross Section and Integral Data," International Conference on the Physics of Nuclear Science and Technology, October 5-8, 1998, Islandia Radisson Hotel, Long Island, New York.

NL99b N. M. Larson, *ORELA Realistic Resolution Function for SAMMY*, in preparation.

NL99c N. M. Larson, *RPI Resolution Function for SAMMY*, in preparation.

NL01 N. M. Larson, *Multiple-Scattering Corrections to Capture and Fission Yields*, in preparation.

NL01a N. M. Larson, *Multigroup Cross Sections in the Bonarenko Narrow-Resonance Approximation, as implemented in SAMMY*, in preparation.

54. P. E. Koehler et al., "Resonance Neutron Capture and Transmission Measurements and the Stellar Neutron Capture Cross Sections of ^{134}Ba and ^{136}Ba," *Phys. Rev. C* **54**, 1463–1477 (1996).

55. O. Bouland, H. Derrien, N. M. Larson, and L. C. Leal, "R-Matrix Analysis of the ^{240}Pu neutron Cross Sections in the Thermal to 5700-eV Energy Range," *Nucl. Sci. Eng.* **127** 105-129 (1997). Also published as ORNL/TM-13450, August 1997.

56. L. C. Leal, N. M. Larson, D. C. Larson, and D. M. Hetrick, "R-Matrix Evaluation of ^{28}Si, ^{29}Si, ^{30}Si up to 1.8 MeV," *International Conference on Nuclear Data for Science and Technology*, May 19–24, 1997, Trieste, Italy.

57. L. C. Leal, H. Derrien, and N. M. Larson, "Statistical Properties of the *s*-Wave Resonances of ^{235}U," *International Conference on Nuclear Data for Science and Technology*, May 19–24, 1997, Trieste, Italy.

58. D. M. Hetrick, D. C. Larson, N. M. Larson, L. C. Leal, and S. J. Epperson, *Evaluation of $^{28, 29, 30}$Si Neutron Induced Cross Sections for ENDF/B-VI*, ORNL/TM-11825, April 1997.

59. L. C. Leal, H. Derrien, N. M. Larson, R. Q. Wright, *R-Matrix Analysis of ^{235}U Neutron Transmission and Cross Sections in the Energy Range 0 to 2.25 keV*, ORNL/TM-13516 (November 1997). Also *Nucl. Sci. and Eng.* **131** 230 (February 1999).

60. P. E. Koehler et al., "New Neutron Capture and Transmission Measurements for ^{134,136}ba at Orela and Their Impact on *S*-process Nucleosynthesis Calculations," *Nucl. Phys. A* **621**, 258c-261c (1997).

61. K. H. Guber, R. R. Spencer, P. E. Koehler, and R. R. Winters, "A BaF_2 detector system for (n,γ) cross section measurements at ORELA," *Nucl. Phys. A* **621**, 254c–257c (1997).

62. K. H. Guber, R. R. Spencer, P. E. Koehler, and R. R. Winters, "Measurements of ^{142,144}Nd (n,γ) cross sections at ORELA for astrophysical *s*-process studies," *Nucl. Phys. A* **621**, 266c (1997).

63. K. H. Guber, R. R. Spencer, P. E. Koehler, and R. R. Winters, "New ^{142,144}Nd(n,γ) Cross Sections and the *s*-process Origin of the Nd Anomalies in Presolar Meteoric Silicon Carbide Grains," *Phys. Rev. Letters* **78**, 2704–2707 (1997).

64. Y. Danon, C. J. Werner, G. Youk, R. C. Block, R. E. Slovacek, and N. C. Francis, "Neutron Total Cross-Section Measurements and Resonance Parameter Analysis of Holmium, Thulium, and Erbium from 0.001 to 20 eV," *Nucl. Sci. Eng.* **128**, 61–69 (1998).

65. L. C. Leal, R. O. Sayer, and N. M. Larson, "R-Matrix Evaluation of ^{16}O Neutron Cross Sections up to 6.3 MeV," November 1998 ANS Conference in Washington, D. C.

66. W. I. Furman, "Fission Channels and Modes," 199 Frederic Joliot / Otto Hanh Spring Session on Neutron Data Measurements and Evaluation, May 17-21, 1999, Geel, Belgium.

67. P. E. Koehler, R. R. Spencer, K. H. Guber, R. R. Winters, S. Raman, J. A. Harvey, N. W. Hill, J. C. Blackmon, D. W. Bardayan, D. D. Larson, T. A. Lewis, D. E. Pierce, and M. S. Smith, "High resolution neutron capture and transmission measurements on ^{137}Ba and their impact on the interpretation of meteoric barium anomalies," *Phys. Rev.C Rapid Communications* **57**, 1558-1561 (1998).

68. H. Derrien, J. A. Harvey, N. M. Larson, L. C. Leal, and R.Q. Wright, "Neutron Total Cross Sections of ^{235}U from Transmission Measurements in the Energy Range 2 keV to 300 keV and Statistical Model Analysis of the Data," ORNL/TM-2000/129, May 2000.

INTERNAL DISTRIBUTION

1. B. L. Broadhead
2. H. Derrien
3. F. C. Difilippo
4. M. E. Dunn
5. C. Y. Fu
6. N. M. Greene
7. K. Guber
8. F. B. Guimaraes
9. J. A. Harvey
10. C. M. Hopper
11. D. T. Ingersoll
12. P. E. Koehler
13. M. A. Kuliasha
14. D. C. Larson
15-19. N. M. Larson
20. L. C. Leal
21. C. V. Parks
22. S. Raman
23. R. W. Roussin
24. R. O. Sayer
25. M. S. Smith
26. R. R. Spencer
27. T. E. Valentine
28. R. M. Westfall
29. J. E. White
30. R. R. Winters
32-33. RSICC
33. Laboratory Records for submission to OSTI
34. Laboratory Records, ORNL-RC
Central Research Library

EXTERNAL DISTRIBUTION

35. S. M. Austin, NSCL/Cyclotron Lab, Michigan State University, East Lansing, MI 48824
36. C. Bastien, Central Bureau for Nuclear Measurements, Steenweg op Retie, 2240 Geel, Belgium
37. P. Blaise, DER/SPRC/LEPH, Batiment 230, Centre d'Etudes de CADARACHE, 13108 Saint Paul-lez-Durance, France
38. R. Block, Gaerttner LINAC Laboratory, Department of Environmental and Energy Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
39. O. Bouland, DER/SPRC/LEPH, Batiment 230, Centre d'Etudes de CADARACHE, 13108 Saint Paul-lez-Durance, France
40. A. Brusegan, Central Bureau for Nuclear Measurements, Steenweg op Retie, 2240 Geel, Belgium
41. David Buchan P41 E1, Pickering Nuclear Generating Station, Ontario Hydro,1675 Montgomery Park Rd., Pickering, Ontario CANADA L1V 2R5
42. J. Burke, Gaerttner LINAC Laboratory, Department of Environmental and Energy Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
43. D. Cabrilla, U.S. Department of Energy, EM-66, Clover Leaf, Room 1199, 19901 Germantown Road, Germantown, MD 20874-1290
44. D. E. Carlson, Reactor and Plant System Branch, Division of System Research, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission, MS T-10 G6, RM T-10, I7, Washington, DC 20555-0001
45. R. F. Carlton, Department of Chemistry and Physics, Middle Tennessee State University, Murfreesboro, TN 37132
46. E. Caro, Lockheed Martin Corporation, P.O. Box 1072, Schenectady, N. Y. 12301-1072

47. Daniel L. Castro, Physics Education and Engineering Education Departments, Instruction and Training Faculty, California Community Colleges, 1120 Cotton Street, San Diego, California 92102-3639.
48. M. Chadwick,T-2, MS B243, Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545
49. F. Corvi, Central Bureau for Nuclear Measurements, Steenweg op Retie, 2240 Geel, Belgium
50. D. E. Cullen, MS L-298, Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA 94550
51. Y. Danon, Gaerttner LINAC Laboratory, Department of Environmental and Energy Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
52. R. L. Dintaman, U.S. Department of Energy, DP-13, Washington, DC 20585
53. C. Dunford, Bldg 197D, National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973
54. J. R. Felty, U.S. Department of Energy, DP-311, Washington DC 20585
55. P. Finck, Argonne National Laboratory, Reactor Analysis Division, Bldg 208, Argonne, IL 60439
56. E. Fort, DER/SPRC/LEPH, Batiment 230, Centre d'Etudes de CADARACHE, 13108 Saint Paul-lez-Durance, France
57. N. Francis, Gaerttner LINAC Laboratory, Department of Environmental and Energy Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
58. C. M. Frankle, NIS-6, MS J562, Los Alamos National Laboratory, Los Alamos, NM 87545
59. S. C. Frankle, X-CI, MS F663, Los Alamos National Laboratory, Los Alamos, NM 87545
60. F. Froehner, Kernforschungszentrum Karlsruhe, Institut fur Neutronenphysik und Reacktortechnik, Postfach 336 40, D-76021 Karlsruhe, Germany
61. W. Furman, Frank Laboratory of Neutron Physics, JINR, Dubna, Russia
62. S. Ganesan, Theoretical Physics Division, Central Complex, 5th Floor, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085 INDIA
63. C. Gould, Physics Dept., North Carolina State University, Box 8202, Raleigh, NC 27695-8202
64. F. Gunsing, Centre D'Etudes De Saclay, F-Saclay - 91191 GIF-SUR-YVETTE Cedex, France
65. G. M. Hale, T-2, MS B243, Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545
66. A. Hasagawa, Nuclear Data Center, Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki-ken 319-11, Japan
67. R. N. Hwang, Argonne National Laboratory, Reactor Analysis Division, Bldg 208, Argonne, IL 60439
68. R. P. Jacqmin, DER/SPRC/LEPH, Batiment 230, Centre d'Etudes de CADARACHE, 13108 Saint Paul-lez-Durance, France
69. N. Janeva, Bulgarian Academy of Sciences, 72, Boul, Tzarigradsko shosse, Sofia 1784, Bulgaria
70. L. Lois, 08 E23, U.S. Nuclear Regulatory Commission, 11555 Rockville Pike, Rockville, MD 20852-2746
71. G. Leinweber, Gaerttner LINAC Laboratory, Department of Environmental and Energy Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
72. R. Little, X-CI, MS F663, Los Alamos National Laboratory, Los Alamos, NM 87545
73. M. Lubert, Gaerttner LINAC Laboratory, Department of Environmental and Energy Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
74. C. Lubitz, Knolls Atomic Power Laboratory, P. O. Box 1072, Schenectady, NY 12301
75. R. E. MacFarlane,T-2, MS B243, Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545-1663
76. C. Mounier, CEN Saclay, DMT/SERMA/LENR, 91191 Gif Sur Yvette Cedex, France

77. M. C. Moxon, 3 Hyde Copse, Marcham, Abingdon, Oxfordshire, England
78. S. F. Mughabghab, Brookhaven National Laboratory, Advanced Technology, Building 197d, Upton, NY 11973-5000
79. D. Muir, IAEA Nuclear Data Section, Wagramerstr. 5, P. O. Box 100, A-1400 Wien, Austria
80. C. W. Nilson, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission, Mail Stop TWFN 9-F-33, Washington, DC 20555
81. J. C. Nimal, DRN/DMT/SERMA, CEA Saclay, bat 470, F-91191 Gif sur Yvette Cedex, France
82. C. Nordborg, OECD/NEA, Le Seine St-Germain 12, Boulevard Iles, 92130 Issy-les-Moulineaux, France
83. A. Nouri, OECD/NEA Data Bank, Le Seine Saint Germain, 12, Bd des Iles, 92130 Issy-Les-Moulineaux (France)
84. S. Y. OH, Nuclear Data Evaluation Lab., Korea Atomic Energy Research Institute, P. O. Box 105, Yusung, Taejon, 305-600 Korea
85. A. Popov, Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, RU-141980 Dubna, Moscow Region, Russia
86. C. Raepsaet, CEN Saclay, DMT/SERMA/LEPP, 91191 Gif Sur Yvette Cedex, France
87. M. Salvatores, DRN/P, Batiment 707, C. E. CADARACHE, 13108 Saint Paul-lez-Durance, France
88. E. Sartori, OECD/NEA, Le Seine St-Germain 12, Boulevard Iles, 92130 Issy-les-Moulineaux, France
89. O. A. Shcherbakov, Petersburg Nuclear Physics Institute, 188 350 Gatchina, Leningrad District, Russia
90. R. Shelley, Central Bureau for Nuclear Measurements, Steenweg op Retie, 2240 Geel, Belgium
91. K. Shibata, Nuclear Data Center, Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki-ken 319-11, Japan
92. Mihaela Sin, Nuclear Physics Department, Bucharest University, P.O. BOX MG-11, RO-76900 Bucharest-Magurele, ROMANIA
93. R. Slovacek, Gaerttner LINAC Laboratory, Department of Environmental and Energy Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
94. A. B. Smith, TD 362 D216, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439
95. D. L. Smith, TD 360 L106, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439
96. H. Takano, Nuclear Data Center, Japan Atomic Energy Research Institute, Tokai-mura, Ibaraki-ken 319-11, Japan
97. J.J. Wagschal, Racah Institute of Physics, The Hebrew University of Jerusalem, 91904, Jerusalem, ISRAEL
98. H. Weigmann, Central Bureau for Nuclear Measurements, Steenweg op Retie, 2240 Geel, Belgium
99. J. P. Weinman, Lockheed Martin Corporation, P.O. Box 1072, Schenectady, N. Y. 12301-1072
100. C. J. Werner, Los Alamos National Laboratory, Los Alamos, NM 87545
101. R. M. White, Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA 94550
102. M. Williams, Nuclear Science Center, Louisiana State University, Baton Rouge, LA 70803
103. P. G. Young, MS B243 T-16 Nuclear Physics, Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545